L Number	Hits	Search Text	DB	Time stamp
1	1	("5767322").PN.	USPAT;	2002/09/05 18:20
			US-PGPUB	
2	34	cumene adj hydroperoxide adj water	USPAT;	2002/09/05 18:24
			US-PGPUB	
3	28	cumene adj hydroperoxide adj mixture	USPAT;	2002/09/05 18:24
			US-PGPUB	
4	8	cumene adj hydroperoxide adj composition	USPAT;	2002/09/05 18:24
İ			US-PGPUB	
5	35	(cumene adj hydroperoxide adj mixture) or	USPAT;	2002/09/05 18:25
		(cumene adj hydroperoxide adj composition)	US-PGPUB	
6	32	((cumene adj hydroperoxide adj mixture) or	USPAT;	2002/09/05 18:25
		(cumene adj hydroperoxide adj composition))	US-PGPUB	
		and (water or H2O)		

Welcome to STN International! Enter x:x

LOGINID:ssspta1204jxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
        Apr 08
                 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS
         Apr 09
         Apr 09
                 ZDB will be removed from STN
NEWS
         Apr 19
NEWS 5
                 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
         Apr 22
                 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 6
NEWS
         Apr 22
                 BIOSIS Gene Names now available in TOXCENTER
NEWS 8
         Apr 22
                Federal Research in Progress (FEDRIP) now available
NEWS 9
         Jun 03
                New e-mail delivery for search results now available
        Jun 10
NEWS 10
                MEDLINE Reload
                PCTFULL has been reloaded
NEWS 11
        Jun 10
NEWS 12
        Jul 02
                FOREGE no longer contains STANDARDS file segment
        Jul 22 USAN to be reloaded July 28, 2002;
NEWS 13
                 saved answer sets no longer valid
NEWS 14
         Jul 29
                 Enhanced polymer searching in REGISTRY
NEWS 15
         Jul 30
                 NETFIRST to be removed from STN
NEWS 16
        Aug 08
                 CANCERLIT reload
NEWS 17
         Aug 08
                 PHARMAMarketLetter (PHARMAML) - new on STN
NEWS 18
         Aug 08
                 NTIS has been reloaded and enhanced
NEWS 19
        Aug 19
                Aquatic Toxicity Information Retrieval (AQUIRE)
                 now available on STN
NEWS 20
        Aug 19
                 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21
        Aug 19
                 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22
                 Sequence searching in REGISTRY enhanced
         Aug 26
NEWS 23
        Sep 03 JAPIO has been reloaded and enhanced
NEWS EXPRESS
             February 1 CURRENT WINDOWS VERSION IS V6.0d,
              CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
              AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
              STN Operating Hours Plus Help Desk Availability
NEWS HOURS
NEWS INTER
              General Internet Information
NEWS LOGIN
              Welcome Banner and News Items
NEWS PHONE
              Direct Dial and Telecommunication Network Access to STN
NEWS WWW
              CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 17:20:54 ON 05 SEP 2002

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

0.21

0.21

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 17:21:16 ON 05 SEP 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 5 Sep 2002 VOL 137 ISS 10 FILE LAST UPDATED: 4 Sep 2002 (20020904/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.40 0.61

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:21:28 ON 05 SEP 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 4 SEP 2002 HIGHEST RN 446821-48-3 DICTIONARY FILE UPDATES: 4 SEP 2002 HIGHEST RN 446821-48-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s cumene hydroperoxide/cn

L1 1 CUMENE HYDROPEROXIDE/CN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 80-15-9 REGISTRY

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

```
OTHER CA INDEX NAMES:
     Hydroperoxide, .alpha.,.alpha.-dimethylbenzyl (8CI)
OTHER NAMES:
CN
     .alpha.,.alpha.-Dimethylbenzyl hydroperoxide
     .alpha.-Cumene hydroperoxide
CN
CN
     .alpha.-Cumyl hydroperoxide
CN
     1-Methyl-1-phenylethyl hydroperoxide
CN
     2-Hydroperoxy-2-phenylpropane
CN
     2-Phenyl-2-propyl hydroperoxide
CN
     7-Cumyl hydroperoxide
CN
     CHP 158
CN
     Cumen hydroperoxide
CN
     Cumene hydroperoxide
     Cumenyl hydroperoxide
CN
     Cumyl hydroperoxide
CN
CN
     Hyperiz
     Isopropylbenzene hydroperoxide
CN
CN
     Kayacumene H
CN
     Percumyl H
     Percumyl H 80
CN
CN
     R 239A
CN
     Trigonox K 80
CN
     Trigonox R 239A
CN
     Trigonox R 239R
FS
     3D CONCORD
DR
     79568-78-8
MF
     C9 H12 O2
CI
     COM
                   AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS,
LC
     STN Files:
       BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*,
       DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*,
       HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2,
       USPATFULL, VTB
          (*File contains numerically searchable property data)
     Other Sources: DSL**, EINECS**, TSCA**
          (**Enter CHEMLIST File for up-to-date regulatory information)
   о-он
Me-C
     - Me
   Ph
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
             4686 REFERENCES IN FILE CA (1967 TO DATE)
              39 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             4690 REFERENCES IN FILE CAPLUS (1967 TO DATE)
               28 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
=> s cumene hydroperoxide
           657 CUMENE
          5406 HYDROPEROXIDE
              4 HYDROPEROXIDES
          5406 HYDROPEROXIDE
                  (HYDROPEROXIDE OR HYDROPEROXIDES)
L2
            25 CUMENE HYDROPEROXIDE
                  (CUMENE (W) HYDROPEROXIDE)
```

=> s 12 and water

2160 WATER

78 WATERS

2238 WATER

(WATER OR WATERS)

L3 0 L2 AND WATER

=> s 12 and h20

244 H20

L4 0 L2 AND H20

=> d scan ;2

L4 HAS NO ANSWERS

2 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d scan 12

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C9 H12 O2 . C4 H9 N O

CM 1

CM 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-phenylethyl, sodium salt (9CI)

MF C9 H12 O2 . Na

Na

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-(4-bromophenyl)-1-methylethyl (9CI)

MF C9 H11 Br O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-phenylethyl (9CI)

MF C9 H12 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Formamide, compd. with 1-methyl-1-phenylethyl hydroperoxide (1:1) (9CI)

MF C9 H12 O2 . C H3 N O

CM 1

$H_2N-CH=0$

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C12 H18 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C12 H18 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-(3-chlorophenyl)-1-methylethyl (9CI)

MF C9 H11 Cl O2

CI COM

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Hydroperoxide, 1-methyl-1-phenylethyl, potassium salt (9CI)

MF C9 H12 O2 . K

K

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 4-(1-hydroperoxy-1-methylethyl)- (9CI)

MF C10 H12 O4

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-[3-(1-methylethyl)phenyl]ethyl (9CI)

MF C12 H18 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Acetamide, compd. with 1-methyl-1-phenylethyl hydroperoxide (1:1) (9CI)

MF C9 H12 O2 . C2 H5 N O

CM 1

CM 2

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-phenylethyl, lithium salt (9CI)
MF C9 H12 O2 . Li

• Li

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-(4-chlorophenyl)-1-methylethyl (9CI)

MF C9 H11 Cl O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Pitch, phenol manuf. cumene hydroperoxide oxidn.
- MF Unspecified
- CI MAN, CTS
- *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
- L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Hydroperoxide, 1-(3,4-dichlorophenyl)-1-methylethyl (9CI)

MF C9 H10 Cl2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-[4-(1,1-dimethylethyl)phenyl]-1-methylethyl (9CI)

MF C13 H20 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN Peroxide, bis(1-methyl-1-phenylethyl) (9CI) ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT MF C18 H22 O2 CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Formamide, N,N-dimethyl-, compd. with 1-methyl-1-phenylethyl hydroperoxide (1:1) (9CI)

MF C9 H12 O2 . C3 H7 N O

CM 1

CM 2

$$^{\text{CH}_3}$$

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-(4-nitrophenyl)ethyl (9CI)

MF C9 H11 N O4

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-(4-methylphenyl)ethyl (9CI)

MF C10 H14 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C13 H19 Cl O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-(2-chlorophenyl)-1-methylethyl (9CI)

MF C9 H11 Cl O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-(2-methylphenyl)ethyl (9CI)

MF C10 H14 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroperoxide, 1-methyl-1-[4-(1-methylethyl)phenyl]ethyl (9CI)

MF C12 H18 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 22.34 22.95

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 17:22:28 ON 05 SEP 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 5 Sep 2002 VOL 137 ISS 10 FILE LAST UPDATED: 4 Sep 2002 (20020904/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d his

(FILE 'HOME' ENTERED AT 17:20:54 ON 05 SEP 2002)

FILE 'CAPLUS' ENTERED AT 17:21:16 ON 05 SEP 2002

FILE 'REGISTRY' ENTERED AT 17:21:28 ON 05 SEP 2002

L1 1 S CUMENE HYDROPEROXIDE/CN

L2 25 S CUMENE HYDROPEROXIDE

L3 0 S L2 AND WATER L4 0 S L2 AND H20

FILE 'CAPLUS' ENTERED AT 17:22:28 ON 05 SEP 2002

=> s l1 and weight percent water 4694 L1

```
7555 WEIGHTS
         93397 WEIGHT
                 (WEIGHT OR WEIGHTS)
       1272657 WT
         94563 WTS
       1321531 WT
                 (WT OR WTS)
       1348119 WEIGHT
                 (WEIGHT OR WT)
         67923 PERCENT
          1267 PERCENTS
         68985 PERCENT
                 (PERCENT OR PERCENTS)
       1940411 WATER
        212506 WATERS
       1991062 WATER
                 (WATER OR WATERS)
            32 WEIGHT PERCENT WATER
                 (WEIGHT (W) PERCENT (W) WATER)
T.5
             0 L1 AND WEIGHT PERCENT WATER
=> s l1 (l) (water or h2o)
          4694 L1
       1940411 WATER
        212506 WATERS
       1991062 WATER
                 (WATER OR WATERS)
        918284 H2O
           118 L1 (L) (WATER OR H2O)
L6
=> s cumene?/ti
L7
         2029 CUMENE?/TI
=> s 16 and 17
            10 L6 AND L7
=> d ti 1-10
     ANSWER 1 OF 10 CAPLUS COPYRIGHT 2002 ACS
TI
     Process for separating phenol from a mixture comprising at least
     hydroxyacetone, cumene, water and phenol
L8
     ANSWER 2 OF 10 CAPLUS COPYRIGHT 2002 ACS
     Preparation of environmentally safe, water-diluted cumene
TI
     hydroperoxide solutions
     ANSWER 3 OF 10 CAPLUS COPYRIGHT 2002 ACS
TI
     Procedure for the recovery of cumene hydroperoxide from
     hydroperoxide-containing, phenol-manufacture process waste water by
     extraction with cumene
L8
     ANSWER 4 OF 10 CAPLUS COPYRIGHT 2002 ACS
     Water-alkaline emulsion cumene oxidation process
TI
L8
     ANSWER 5 OF 10 CAPLUS COPYRIGHT 2002 ACS
TI
     Reliability and hazards analysis of a cumene hydroperoxide plant
L8
     ANSWER 6 OF 10 CAPLUS COPYRIGHT 2002 ACS
ΤI
     Oxidation of cumene in the presence of water additives
     ANSWER 7 OF 10 CAPLUS COPYRIGHT 2002 ACS
L8
     Chromatographic determination of water and phenol in products from the
ΤI
     manufacture of phenol and acetone by the cumene hydroperoxide
```

87965 WEIGHT

process

```
ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS
Ь8
     Cumene hydroperoxide
ΤI
     ANSWER 9 OF 10 CAPLUS COPYRIGHT 2002 ACS
1.8
     Study of intermolecular interactions in the cumene
TI
     hydroperoxide-water system by the proton magnetic resonance method
L8
     ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS
     Study of the decomposition of cumene hydroperoxide in the
TI
     presence of different inhibitors during production of butadiene-styrene
     rubbers
=> d ibib abs hitstr 1-10
     ANSWER 1 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER:
                         2002:429321 CAPLUS
DOCUMENT NUMBER:
                         136:403494
TITLE:
                         Process for separating phenol from a mixture
                         comprising at least hydroxyacetone, cumene,
                         water and phenol
INVENTOR(S):
                         Schwarz, Christoph; Weber, Mark; Tanger, Uwe; Korte,
                         Hermann-Josef; Ullrich, Jochen
PATENT ASSIGNEE(S):
                         Phenolchemie G.m.b.H. & Co. K.-G., Germany
SOURCE:
                         U.S. Pat. Appl. Publ., 9 pp.
                         CODEN: USXXCO
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                  KIND DATE
                                          APPLICATION NO. DATE
                                           -----
     US 2002066661 A1
                            20020606
                                          US 2001-970856 20011005
     WO 2002046133
                     A1 20020613
                                          WO 2001-EP14029 20011130
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:
                                       DE 2000-10060505 A 20001206
     Phenol is sepd. from a mixt. contg. hydroxyacetone, cumene, H2O and
     phenol, by fractionating the mixt. in a process with a fractional distn.
     step and a phase sepn. step to provide a single phenol fraction contg.
     <300 ppm of hydroxyacetone. In the work-up by distn. of cleavage product
     mixts., the hydroxyacetone can be removed from the cleavage product mixt.
     together with a phenol fraction from which the hydroxyacetone has to be
     removed. A process can be used for purifying cleavage product mixts.
     obtained in the cleavage of alkylaryl hydroperoxides such as cumene
     hydroperoxide. The process allows sepn. of phenol and acetone from mixts.
     obtained in the cleavage of cumene hydroperoxide.
IT
     80-15-9, Cumene hydroperoxide
    RL: CAT (Catalyst use); USES (Uses)
        (process for sepg. phenol from a mixt. comprising at least
```

hydroxyacetone, cumene, water and phenol)

Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

RN

CN

80-15-9 CAPLUS

L8 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:2

2002:220548 CAPLUS

DOCUMENT NUMBER:

136:264830

TITLE:

Preparation of environmentally safe, water-diluted

cumene hydroperoxide solutions

INVENTOR(S):
PATENT ASSIGNEE(S):

Henry, Keith E.; Aiken, John E. Aristech Chemical Corporation, USA

SOURCE:

PCT Int. Appl., 16 pp.

DOCUMENT TYPE:

CODEN: PIXXD2 Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2002022570 A2 20020321 WO 2001-US28123 20010904
WO 2002022570 A3 20020704

W: AU, CA, JP, KR, MX, NO, RU

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,

PT, SE, TR

AU 2001088913 A5 20020326 AU 2001-88913 20010904 PRIORITY APPLN. INFO.: US 2000-660099 A 20000912 WO 2001-US28123 W 20010904

The use of water, rather than cumene, as a more environmentally acceptable diluent for purified cumene hydroperoxide (CHP) solns. is described. From 1-6% water can be used to dil. purified CHP solns., thus reducing or eliminating the use of the hazardous compd. cumene as a diluent. This method and the CHP-water solns. significantly reduce or eliminate the hazardous emissions problems encountered with the use of cumene as a diluent and make CHP solns. more environmentally acceptable to produce, transport, and use. Water as a diluent also depresses the f.p. of the resultant soln., thus enabling year-round use of higher-concn. CHP solns. Water-dild. CHP solns. also reduce cumene-related impurities in finished products made from them.

IT 80-15-9, Cumene hydroperoxide

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(prepn. of safe water-dild. cumene hydroperoxide solns.)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 2000:188382 CAPLUS

DOCUMENT NUMBER: 132:209457

TITLE:

Procedure for the recovery of cumene

hydroperoxide from hydroperoxide-containing,

phenol-manufacture process waste water by extraction

with cumene

INVENTOR(S):

Hofmann, Guenter; Pester, Rolf; Bartkowiak, Horst

Domo Caproleuna G.m.b.H., Germany

SOURCE:

Ger., 6 pp. CODEN: GWXXAW

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT NO. KIND DATE APPLICATION NO. DATE -----_____ DE 19846508 C1 20000323 DE 1998-19846508 19981009 EP 997456 A1 20000503 EP 1999-119594 19991002

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.:

DE 1998-19846508 19981009

Cumene hydroperoxide is recovered from hydroperoxide-contg., phenol-manuf. process waste water by extn. of the water with cumene (cumol) which is formed during phenol manuf. The waste water resulting after the extn. contains only traces of cumene hydroperoxide and exhibits almost no removal of the residual Me hydroperoxide.

IT 80-15-9P, Cumene hydroperoxide

> RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PREP (Preparation); PROC (Process)

(procedure for the recovery of cumene hydroperoxide from hydroperoxide-contg. phenol-manuf. process waste water by extn. with cumol)

RN80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

0-- ОН Me-C-Me Ph

REFERENCE COUNT:

1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1998:116085 CAPLUS

DOCUMENT NUMBER:

TITLE:

128:129491

Water-alkaline emulsion cumene oxidation

process

INVENTOR(S):

Zakoshansky, Vladimir Michailo; Griaznov, Andrei K.; Vasilieva, Irina Ivanovna; Fulmer, John William;

Kight, William Dale

PATENT ASSIGNEE(S):

General Electric Co., USA

SOURCE:

Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE 100 ----------------A1 19980107 EP 816335 EP 1997-304341 19970620

EP 816335 В1 20011031 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI US 1996-670304 19960627 US 5767322 19980616 ES 1997-304341 ES 2163102 20020116 19970620 Т3 CN 1997-114047 CN 1173491 Α 19980218 19970624 CN 1088059 В 20020724 JP 1997-167816 JP 10087609 A2 19980407 19970625 US 5908962 US 1998-20395 Α 19990601 19980209 A 19960627 PRIORITY APPLN. INFO.: US 1996-670304

AB Greater efficiency in the title process using a cascade of reactors is obtained by splitting the reactor cascade into 2 stages with the 1st stage utilizing NH4NaCO3 as the active carbonate in the stage contg. .ltoreq.18% cumene hydroperoxide (I) and using Na2CO3 as the active carbonate in the stage contg. .gtoreq.18% I. By directly injecting ammonia into a recycle stream org. acids are efficiently neutralized. A counter current water wash of the 2nd stage also increases process efficiency by scrubbing out unwanted impurities. Control of pH in the process improves efficiency and reduces impurity levels.

IT 80-15-9P, Cumene hydroperoxide

RL: IMF (Industrial manufacture); PREP (Preparation) (water-alk. emulsion cumene oxidn. process with good efficiency)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

L8 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1986:429162 CAPLUS

DOCUMENT NUMBER: 105:29162

TITLE: Reliability and hazards analysis of a cumene

hydroperoxide plant

AUTHOR(S): Arendt, J. S.; Casada, M. L.; Rooney, J. J. CORPORATE SOURCE: JBF Assoc. Inc., Knoxville, TN, 37932, USA SOURCE: Plant/Oper. Prog. (1986), 5(2), 97-102

CODEN: POPPDE; ISSN: 0278-4513

DOCUMENT TYPE: Journal LANGUAGE: English

AB An anal. of reliability and risk of a cumene hydroperoxide [
80-15-9] plant led to conclusions that call for the updating of
the existing emergency procedures dealing with the oxidizers, inspections
and testing of important safety equipment on a regular basis, shortening
the closure time delay of the main process air valve in case of a power
outage, and a modification of the existing emergency procedures for the
diesel cooling water system.

L8 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:67930 CAPLUS

DOCUMENT NUMBER: 100:67930

TITLE: Oxidation of cumene in the presence of water

additives

AUTHOR(S): Golysheva, G. P.; Ionova, M. V.; Il'ina, T. A.;

Vasil'ev, V. F.

CORPORATE SOURCE: Vses. Nauchno-Issled. Inst. Org. Sint.,

Novokuibyshevsk, USSR

SOURCE: Neftepererab. Neftekhim. (Moscow) (1983), (12), 31

CODEN: NNNSAF; ISSN: 0028-1190

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB Addn. of H2O to a cumene oxidn. system increased the rate of cumene

hydroperoxide formation but lowered the selectivity.

IT 80-15-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, effect of water on)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

O-OH | Me-C-Me | Ph

L8 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:624444 CAPLUS

DOCUMENT NUMBER: 99:224444

TITLE: Chromatographic determination of water and phenol in

products from the manufacture of phenol and acetone by

the cumene hydroperoxide process

AUTHOR(S): Bruk, A. Yu.; Gaishun, K. A.; Markova, V. A.

CORPORATE SOURCE: Grozn. KhZ, Grozny, USSR

SOURCE: Neftepererab. Neftekhim. (Moscow) (1983), (10), 23-4

CODEN: NNNSAF; ISSN: 0028-1190

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB H2O and PhOH were detd. by gas chromatog. with thermal-cond. and flame-ionization detectors, resp. Various products were analyzed, such as Me2CO, phenol-formaldehyde resin, Syntan 2 tanning agent, and the reaction mass from the decompn. of cumene hydroperoxide. The sepn. was carried out at 130.degree. on a 50 .times. 0.3-cm column packed with Polysorb 1 coated

with 5 wt.% Tween 80.

IT **80-15-9D**, decompn. products RL: ANST (Analytical study)

(phenol and water detn. in, gas chromatog.)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

O-OH | Me-C-Me | Ph

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:144912 CAPLUS

DOCUMENT NUMBER: 96:144912

TITLE: Cumene hydroperoxide

INVENTOR(S): Franke, Christiane; Fuhrmann, Guenther; Haase, Bernd;

Hager, Werner; Hofmann, Rolf; Naumann, Hans Joachim;

Raue, Bernd

PATENT ASSIGNEE(S): VEB Leuna-Werke "Walter Ulbricht", Ger. Dem. Rep.

SOURCE: Ger. (East), 10 pp.

CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DD 151000 T 19810930 DD 1979-212412 19790423 cumene [98-82-8] Is oxidized to prep. cumene hydroperoxide (I) AB 80-15-9], and the unreacted cumene is sepd. by distn., washed with water to remove org. acids (esp. HCO2H), and recycled to the oxidn. step. Addnl. I is extd. from the water with cumene. The method increases the yield of I, decreases the formation of by-products, and minimizes the deposition of insol. materials on surfaces in the app. The I is used to prep. phenol and acetone. Thus, 54,100 parts oxidn. products contg. I 20.6, PhCMe2OH 1.4, and PhAc 0.19% was distd. to sep. 11,000 parts I contg. <100 ppm org. acids, and the cumene (contg. 110 parts org. acid, calcd. as HCO2H) was washed with 1600 parts water , mixed with 870 parts cumene and 1.9 parts 15% aq. NaOH, and recycled to the oxidn. step. The water was extd. with 200 parts cumene to recover 8 parts I, giving waste water contg. <2000 ppm I. The oxidn. and distn. app. required cleaning after 1 yr, compared with 350 h when the recycled cumene was not washed with water.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: DOCUMENT NUMBER:

1977:600365 CAPLUS

87:200365

TITLE:

Study of intermolecular interactions in the cumene hydroperoxide-water system by the

proton magnetic resonance method

AUTHOR(S):

SOURCE:

Markaryan, Sh. A.; Beileryan, N. M.; Grigoryan, S. K.

CORPORATE SOURCE:

Erevan. Gos. Univ., Yerevan, USSR Zh. Fiz. Khim. (1977), 51(9), 2385-7

CODEN: ZFKHA9

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

NMR data indicated that in the title system proton exchange occurs between PhCMe200H (I) and H2O. At 97:3 I-H2O the rate const. for this exchange is 85 s-1. Interactions between the .pi. system of I and H2O also occur.

IT 80-15-9

RL: PRP (Properties)

(interaction of, with water)

RN80-15-9 CAPLUS

Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME) CN

ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:30764 CAPLUS

DOCUMENT NUMBER:

86:30764

TITLE:

Study of the decomposition of cumene

hydroperoxide in the presence of different inhibitors

during production of butadiene-styrene rubbers Titov, A. P.; Papkov, V. N.; Smol'yaninova, T. S.

AUTHOR (S): CORPORATE SOURCE:

USSR

SOURCE:

Zh. Prikl. Khim. (Leningrad) (1976), 49(9), 2041-3

CODEN: ZPKHAB

DOCUMENT TYPE:

Journal

LANGUAGE: Russian

The inhibition of emulsion polymn. initiated by cumene hydroperoxide (I) [80-15-9]-redox system by inhibitors [Na N,N-dimethyldithiocarbamate (II) [128-04-1], NaNO2, p-hydroxydiphenylamine (III) [122-37-2], hydroxylamine (IV) [7803-49-8] N,N-diethylhydroxylamine (V) [3710-84-7], or dibenzylhydroxylamine (VI) [621-07-8]] is due in part to the decompn. of I by these inhibitors and in part to the chain termination reactions in which these inhibitors participate. The foregoing was demonstrated by detg. the kinetics of I decompn. in media modelling the emulsions used in prepn. of SBR. These media contained I, redox system, PhMe (substituted for monomers), and water. The effectiveness of I decompn. decreased in the series: V > III > IV > VI > NaNO2 > II which did not correspond exactly to the effectiveness of arresting the formation of SBR in emulsion copolymns.

=> file merck COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 52.96 75.91 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -6.20 -6.20

FILE 'MRCK' ENTERED AT 17:26:43 ON 05 SEP 2002 COPYRIGHT (C) 1996, 2002 Merck & Co., Inc., Whitehouse Station, N. J.

FILE COVERS FROM LATE 19TH CENTURY TO PRESENT. LAST UPDATE: APRIL 2001

Merck & Co., Inc. cannot be responsible for errors in publication or for any consequences arising from use of the information contained in THE MERCK INDEX ONLINE. Reference to original sources is encouraged.

THE MERCK INDEX ONLINE is a service mark of Merck & Co., Inc., Whitehouse Station, N. J., USA.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l1

L9 0 L1

=> d his

L2

(FILE 'HOME' ENTERED AT 17:20:54 ON 05 SEP 2002)

FILE 'CAPLUS' ENTERED AT 17:21:16 ON 05 SEP 2002

FILE 'REGISTRY' ENTERED AT 17:21:28 ON 05 SEP 2002

L1 1 S CUMENE HYDROPEROXIDE/CN

25 S CUMENE HYDROPEROXIDE

L3 0 S L2 AND WATER L4 0 S L2 AND H20

FILE 'CAPLUS' ENTERED AT 17:22:28 ON 05 SEP 2002

L5 0 S L1 AND WEIGHT PERCENT WATER

L6 118 S L1 (L) (WATER OR H2O)

L7 2029 S CUMENE?/TI

L8 10 S L6 AND L7

FILE 'MRCK' ENTERED AT 17:26:43 ON 05 SEP 2002

L9 0 S L1

=> file beilstein COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.30 76.21 SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -6.20 FILE 'BEILSTEIN' ENTERED AT 17:27:00 ON 05 SEP 2002 COPYRIGHT (c) 2002 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein Chemiedaten & Software GmbH and MDL Information Systems GmbH FILE RELOADED ON APRIL 8, 2002 FILE COVERS 1779 TO 2001. *** FILE CONTAINS 8,128,462 SUBSTANCES *** >>> For the revised summary sheet please see: http://info.cas.org/ONLINE/DBSS/beilsteinss.html <<< >>> PLEASE NOTE: Reaction and substance documents are stored in different file segments. Use separate queries to search for reaction and substance data. When searching for bibliographic information you have the option to chose the file segment. (Use "/XXX.SUB" to search for a bibliographic term in substance documents. To restrict the search to reaction documents use "/XXX.RX".) For additional information see HELP RXS. <<< >>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<< ******************** * PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. * FOR PRICE INFORMATION SEE HELP COST ************************ => s l1 L101 L1 => d aze L10 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL Azeotrope (MCS): Value | Ref. ========+==== => d fpre 'FPRE' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN' The following are valid formats: QRD ----- Query Related Data (IDE plus HIT) IDE ----- Identification of Substance, plus Structure (BRN, MF, LSF, CN, SY, AUN, MW, SO, NTE, LN, RN, BPR, RSI, OS, STR) ALL ----- All Display fields (Lengthy display!) CHE ----- Chemical Data

PHY ----- Physical Data

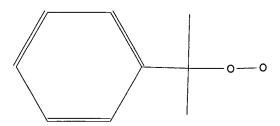
HIT ------ All fields containing hit terms
Hit terms will be highlighted in all IDE fields in the BEILSTEIN file
A maximum of 20 values are displayed in each single property field.
Use DISPLAY F<prop> for FULL format, e.g. FBP instead of BP.
For more information about display formats, and how to display
individual selected properties, enter 'HELP FORMAT' at an arrow
prompt, e.g. => HELP FORMAT.
ENTER DISPLAY FORMAT (QRD):end

=> d ide

L10 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Beilstein Records (BRN): 1908117 Beilstein Pref. RN (BPR): 80-15-9 CAS Reg. No. (RN): 80-15-9 Chemical Name (CN): 1-methyl-1-phenyl-ethyl hydroperoxide, 1-Methyl-1-phenyl-aethylhydroperoxid, .alpha.,.alpha.-dimethylbenzyl hydroperoxide, cumene hydroperoxide, .alpha.-cumyl hydroperoxide Autonom Name (AUN): 1-methyl-1-phenyl-ethyl hydroperoxide Molec. Formula (MF): C9 H12 O2 Molecular Weight (MW): 152.19 Lawson Number (LN): 5240 isocyclic Compound Type (CTYPE): Constitution ID (CONSID): 1754219 Tautomer ID (TAUTID): 1833317 Beilstein Citation (BSO): 3-06-00-01814, 4-06-00-03221, 5-06, 6-06 Entry Date (DED): 1989/06/29

2001/07/25



Update Date (DUPD):

Field Availability:

Code	Name	Occurrence
======	=======================================	=======
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	5
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	4

ED	Entry Date	1
UPD	Update Date	1
ASSM	Association (MCS)	25
BP	Boiling Point	33
CDER	Chemical Derivative	31
DE	Dissociation Exponent	4
DEN	Density (Liquid)	6
DM	Dipole Moment	
DP	Decomposition Point	3 1 8
ECTOX	Ecotoxicology	8
ELCB	Electrochemical Behaviour	1
ESR	ESR Data	2
FINFO	Further Information	1 2 2 1 9
HVAP	Enthalpy of Vaporization	1
IR	Infrared Spectrum	9
LLSM	Liquid/Liquid System (MCS)	8
LUM	Luminescence	8 1 2
MP	Melting Point	
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	20
OTHE	Other Thermochemical Data	1
PHARM	Pharmacological Data	92
RAS	Raman Spectrum	3
RI	Refractive Index	20
RSTR	Related Structure	1
SLB	Solubility (MCS)	3 1
SOLM	Solution Behaviour (MCS)	1
TRAM	Transport Phenomena (MCS)	1
USC	Use of Compound	1
UVS	UV and Visible Spectrum	3
XREF	Crossfile Reference	10

This substance also occurs in Reaction Documents:

Code	Name	Occurrence			
RX	Reaction Documents	301			
RXREA	Substance is Reaction Reactant	276			
RXPRO	Substance is Reaction Product	25			

=> d frxpro

L10 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:

PΧ

Reaction ID: 8753725 Reactant BRN: 2454403

Reactant: Perbuttersaeure-cumolester

Product BRN: 1908117

Product: 1-methyl-1-phenyl-ethyl hydroperoxide

No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 8753725.1
Reaction Classification: Preparation
Reagent: (n-Bu3Sn)20
Solvent: diethyl ether
Time: 30 hour(s)
Temperature: 25 Cel

Reference(s):

```
1. Baj, Stefan; Chrobok, Anna, Syn.Lett.
        , CODEN: SYNLES(5), <2001>, 623 - 624; BABS-6282951
Reaction:
RX
     Reaction ID:
                                    8612643
     Reactant BRN:
                                    1236613
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    1905012, 1908117, 1905601, 969405
     Product:
                                    2-phenyl-propan-2-ol, 1-methyl-1-phenyl-
                                    ethyl hydroperoxide, 2-phenyl-
                                    propionaldehyde, isopropenylbenzene
     Stoichiometric Equation:
                                    1236613 *4
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    8612643.1
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                    Fe(TPFPP)Cl, O2
     Solvent:
                                    various solvent(s)
     Temperature:
                                    100 Cel
     Subject Studied:
                                    Product distribution
     Reaction Type:
                                    Oxidation
     Prototype Reaction:
                                    Further Variations:, reaction times
     Reference(s):
     1. Evans, Steven; Smith, John R. Lindsay, J.Chem.Soc.Perkin Trans.2,
        CODEN: JCPKBH(7), <2000>, 1541 - 1552; BABS-6248901
Reaction:
RX
     Reaction ID:
                                    7160212
     Reactant:
                                    cumene (1-methyl-1-phenyl-ethyl
                                    hydroperoxide containing)
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    7160212.1
     Reaction Classification:
                                    Preparation (half reaction)
     Reagent:
                                    benzoic acid, oxygen
     Note(s):
                                   Handbook
     Reference(s):
     1. Patent: Soc. Usines Chim. Rhone-Poulenc US 2697121 1952
RX
     Reaction RID:
                                    7160212.2
     Reaction Classification:
                                    Preparation (half reaction)
     Reagent:
                                    copper phthalocyanin, oxygen
     Note(s):
                                   Handbook
     Reference(s):
     1. Hock; Kropf, J.Prakt.Chem., CODEN: JPCEAO, <4> 9, <1959>, 173, 176, 184
RX
     Reaction RID:
                                    7160212.3
     Reaction Classification:
                                   Preparation (half reaction)
     Reagent:
                                   NH3, oxygen
     Note(s):
                                   Handbook
     Reference(s):
     1. Patent: Hercules Powder Co. US 2632026 1950
RX
     Reaction RID:
                                   7160212.4
     Reaction Classification:
                                   Preparation (half reaction)
```

aqueous NaOH, oxygen

Reagent:

```
Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Hercules Powder Co. US 2663740 1952
     2. Patent: Distillers Co. DE 924449 1948, DRP/DRBP Org.Chem.
RX
     Reaction RID:
                                    7160212.5
                                    Preparation (half reaction)
     Reaction Classification:
                                    Na2CO3, oxygen
     Reagent:
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: ICI US 2796439 1954
RX
     Reaction RID:
                                    7160212.6
     Reaction Classification:
                                    Preparation (half reaction)
                                    aqueous formaldehyde, oxygen
     Reagent:
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Soc. Usines Chim. Rhone-Poulenc US 2680139 1953
RX
     Reaction RID:
                                    7160212.7
     Reaction Classification:
                                    Preparation (half reaction)
     Reagent:
                                    copper formate, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: ICI US 2820832 1954
RX
     Reaction RID:
                                    7160212.8
     Reaction Classification:
                                    Preparation (half reaction)
     Reagent:
                                    copper benzoate, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: ICI US 2820832 1954
RX
     Reaction RID:
                                    7160212.9
     Reaction Classification:
                                    Preparation (half reaction)
     Reagent:
                                    manganese naphthenate, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Hercules Powder Co. US 2664448 1948
RX
     Reaction RID:
                                    7160212.10
     Reaction Classification:
                                    Preparation (half reaction)
     Reagent:
                                    ethanediyldiimino-tetra-acetic acid, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Edogawa Kagaku Kogyo K.K. US 2861107 1956
Reaction:
RX
     Reaction ID:
                                    7160211
     Reactant BRN:
                                    2037554, 3587191, 1905012
     Reactant:
                                    sulfuric acid, hydrogen peroxide,
                                    2-phenyl-propan-2-ol
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    7160211.1
     Reaction Classification:
                                    Chemical behaviour
     Other Conditions:
                                    180-markierter 2-Phenyl-propan-2-ol
     Note(s):
                                    Handbook
     Reference(s):
```

1. Bassey et al., J.Chem.Soc., CODEN: JCSOA9, <1955>, 2471, 2473

Reaction:

RX

Reaction ID: 7160210 Product BRN: 1908117

Product: 1-methyl-1-phenyl-ethyl hydroperoxide

No. of Reaction Details:

Reaction Details:

Reaction RID: 7160210.1

Reaction Classification: Preparation (half reaction)

Reference(s):

- 1. Patent: Phenolchemie GmbH DE 1668575 1968, Chem. Abstr., 74 (125153m), <1971>
- 2. Richardson; Hodge, J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 4012,4013, 4015
- 3. Antonovskii et al., Kinet.Catal.(Engl.Transl.), CODEN: KICAA8, 6, <1965>, 736, 815
- 4. Patent: Texaco. Devel. Corp. DE 2035504 1970, Chem. Abstr., 76(72223s), <1972>
- 5. Min'kov; Keier, Kinet.Catal. (Engl.Transl.), CODEN: KICAA8, 8, <1967>, 133,134,135
- 6. Min'kov et al., Kinet.Catal.(Engl.Transl.), CODEN: KICAA8, 8, <1967>, 333
- 7. Kulicki; Stec, Rocz.Chem., CODEN: ROCHAC, 50, <1976>, 1075,1076
- 8. Solonko et al., Kinet.Katal., CODEN: KNKTA4, 9, <1968>, 631
- 9. Solomko et al., Kinet.Katal., CODEN: KNKTA4, 9, <1968>, 815
- 10. Ishii et al., Kogyo Kagaku Zasshi, CODEN: KGKZA7, 64, <1961>, 472, Chem.Abstr., 57(7149)
- 11. Tanaka; Imamura, Chem.Lett., CODEN: CMLTAG, <1974>, 1347
- 12. Tsyskovskii et al., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 48, <1975>, 2811,2812-2813, Zh.Prikl.Khim. (Leningrad), CODEN: ZPKHAB, 48, <1975>, 2731
- 13. Choe; Tsutsumi, Nippon Kagaku Zasshi, CODEN: NPKZAZ, 81, <1960>, 582,583, Chem.Abstr., 56(397), <1962>
- 14. Burghardt et al., Zesz.Nauk.Politech.Slask.Chem., CODEN: ZNSCAM, 60, <1972>, 3,4-7,9,10,12-17
- 15. Kulicki, Zesz.Nauk.Politech.Slask.Chem., CODEN: ZNSCAM, 36, <1967>, 1,13,19-24,59,61,62
- 16. Norikov; Salukvadze, Dokl.Phys.Chem.(Engl.Transl.), CODEN: DKPCAG, 203, <1972>, 254
- 17. Choe; Tsutsuni, Nippon Kagaku Zasshi, CODEN: NPKZAZ, 81, <1960>, 582,583-586, Chem.Abstr.(397), <1962>
- 18. Wagner, J.Prakt.Chem., CODEN: JPCEAO, 27, <1965>, 297
- 19. Maruyama et al., Nippon Kagaku Zasshi, CODEN: NPKZAZ, 85, <1964>, 145, Chem. Abstr., 61(13222), <1964>
- Kasmin, J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 35, <1962>, 398, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 35, <1962>, 422, Chem.Abstr., 57(700), <1962>
- 21. Patent: Etienne; Le Berre FR 1239348, Chem.Abstr., 56(3415), <1962>
- 22. Wagner, Z.Chem., CODEN: ZECEAL, 5, <1965>, 73
- 23. Kropf, Justus Liebigs Ann. Chem., CODEN: JLACBF, 637, <1960>, 73,76,92
- 24. Kropf; Knabjohann, Justus Liebigs Ann. Chem., CODEN: JLACBF, 739, <1970>, 95,98,99
- 25. Kulicki; Stec, Rocz.Chem., CODEN: ROCHAC, 45, <1971>, 601,603
- 26. Rouchaud, Bull.Soc.Chim.Belg., CODEN: BSCBAG, 76, <1967>, 171,184 27. Rouchaud, Bull.Soc.Chim.Belg., CODEN: BSCBAG, 76, <1967>, 186
- 28. Gadelle; Clement, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1967>, 1175
- 29. Fukui; Ohkubo, Bull.Chem.Soc.Jpn., CODEN: BCSJA8, 42, <1969>, 312
- 30. Kropf et al., C.R.Seances Acad.Sci.Ser.D, CODEN: CHDDAT, <1968>, 5527

```
RX
     Reaction ID:
                                    7067053
                                    3587191, 2037554, 1855036
     Reactant BRN:
     Reactant:
                                    hydrogen peroxide, sodium hydrogencarbonate,
                                    sulfuric acid, (.alpha.-chloro-isopropyl)-
                                    benzene
     Product BRN:
                                    1908117, 969405
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
     Product:
                                    isopropenylbenzene
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    7067053.1
     Reaction Classification:
                                    Chemical behaviour
     Note(s):
                                    Handbook
     Reference(s):
     1. Ross; Huettel, Chem.Ber., CODEN: CHBEAM, 89, <1956>, 2641, 2643
Reaction:
RX
     Reaction ID:
                                    6731166
     Reactant BRN:
                                    1236613
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    5508788, 1908117, 605842, 1905012
     Product:
                                    cumyl hydrotrioxide, 1-methyl-1-phenyl-ethyl
                                    hydroperoxide, 1-phenyl-ethanone,
                                    2-phenyl-propan-2-ol, ring product
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    6731166.1
     Reaction Classification:
                                    Chemical behaviour
                                    03, 02
     Reagent:
     Solvent:
                                    acetone-d6
     Time:
                                    4 hour(s)
     Temperature:
                                    -40 Cel
     Other Conditions:
                                    further periods of time
     Subject Studied:
                                    Product distribution
     Reference(s):
     1. Pryor, William A.; Ohto, Norio; Church, Daniel F., J.Amer.Chem.Soc.,
        CODEN: JACSAT, 105(11), <1983>, 3614-3622; BABS-5737674
Reaction:
RX
     Reaction ID:
                                    6725969
     Reactant BRN:
                                    1236613
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    1908117, 1905012, 605842, 969616, 635680,
                                    969405
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
                                    2-phenyl-propan-2-ol, 1-phenyl-ethanone,
                                    phenol, propan-2-one, isopropenylbenzene,
                                    acetic acid
     No. of Reaction Details:
                                    1
Reaction Details:
RX
     Reaction RID:
                                    6725969.1
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                    (t-BuO)3Al, t-BuOOH
     Solvent:
                                    benzene
     Time:
                                    3.5 \text{ day}(s)
```

```
Temperature:
     Subject Studied:
                                    Mechanism, Product distribution
     Reference(s):
     1. Stepovik, L. P.; Dodonov, V. A.; Zaburdaeva, E. A., Russ.J.Gen.Chem.,
        CODEN: RJGCEK, 67(1), <1997>, 111-115, Zh.Obshch.Khim., CODEN: ZOKHA4,
        67(1), <1997>, 116-120; BABS-6099494
Reaction:
RX
     Reaction ID:
                                    6674993
     Reactant BRN:
                                    1236613
     Reactant:
                                    oxygen, metal phthalocyaninene,
                                    isopropylbenzene
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
ВX
     Reaction RID:
                                    6674993.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    50 - 150 Cel
     Subject Studied:
                                    Kinetics
     Note(s):
                                    Handbook
     Reference(s):
     1. Hock; Kropf, J. Prakt. Chem., CODEN: JPCEAO, <4> 9, <1959>, 173, 175
Reaction:
RX
     Reaction ID:
                                    6674992
     Reactant BRN:
                                    1236613
     Reactant:
                                    oxygen, lead (IV) oxide, isopropylbenzene
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
                                    1
Reaction Details:
RX
     Reaction RID:
                                    6674992.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    80 Cel
     Subject Studied:
                                   Kinetics
     Note(s):
                                   Handbook
     Reference(s):
     1. Hock; Kropf, J.Prakt.Chem., CODEN: JPCEAO, <4> 6, <1958>, 120
Reaction:
RX
     Reaction ID:
                                    6674991
     Reactant BRN:
                                    1236613
     Reactant:
                                    oxygen, copper, isopropylbenzene
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    6674991.1
     Reaction Classification:
                                   Chemical behaviour
     Temperature:
                                   120 Cel
     Subject Studied:
                                   Kinetics
     Note(s):
                                   Handbook
     Reference(s):

    De Boer et al., Proc.K.Ned.Akad.Wet.Ser.B:Phys.Sci., CODEN: KNWBAA, <B>
```

20 Cel

```
61, <1958>, 170
Reaction:
```

Reaction ID: 6674990 Reactant BRN: 1236613

Reactant: oxygen, copper stearate, isopropylbenzene

Product BRN: 1908117

Product: 1-methyl-1-phenyl-ethyl hydroperoxide

No. of Reaction Details:

Reaction Details:

RX

RX

Reaction RID: 6674990.1

Reaction Classification: Chemical behaviour

Temperature: 100 Cel Note(s): Handbook

Reference(s):

1. George; Rideal; Robertson, Proc.R.Soc.London A, CODEN: PRLAAZ, 185,

<1946>, 288, 297

Reaction:

RX

Reaction ID: 6674989 Reactant BRN: 1236613

Reactant: oxygen, cobalt (II)-stearate,

isopropylbenzene

Product BRN: 1908117

Product: 1-methyl-1-phenyl-ethyl hydroperoxide

No. of Reaction Details:

Reaction Details:

RX

Reaction RID: 6674989.1

Reaction Classification: Chemical behaviour

Temperature: 90 Cel Subject Studied: Kinetics Note(s): Handbook

Reference(s):

1. Kucher, Zh.Fiz.Khim., CODEN: ZFKHA9, 33, <1959>, 617, Chem.Abstr.,

<1959>, 21100

Reaction:

RX

Reaction ID: 6674988 Reactant BRN: 1236613

Reactant: oxygen, cobalt (III)-stearate,

isopropylbenzene

Product BRN: 1908117

Product: 1-methyl-1-phenyl-ethyl hydroperoxide

No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6674988.1

Reaction Classification: Chemical behaviour

Temperature: 90 Cel Subject Studied: Kinetics Note(s): Handbook

Reference(s):

1. Kucher, Zh.Fiz.Khim., CODEN: ZFKHA9, 33, <1959>, 617, Chem.Abstr.,

<1959>, 21100

Reaction:

```
RX
     Reaction ID:
                                    6674987
     Reactant BRN:
                                    1236613
                                    oxygen, barium peroxide, isopropylbenzene
     Reactant:
     Product BRN:
                                    1908117
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     Product:
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    6674987.1
     Reaction Classification:
                                    Chemical behaviour
                                    100 - 140 Cel
     Temperature:
     Subject Studied:
                                    Kinetics
     Note(s):
                                    Handbook
     Reference(s):
     1. Tsunoda; Matsumoto, Tokai technol. J. Japan, 17(1), <1956>, 17
Reaction:
RX
     Reaction ID:
                                    6674985
     Reactant BRN:
                                    390030, 1236613
     Reactant:
                                    oxygen, anthraquinone, isopropylbenzene
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    6674985.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    15 Cel
     Subject Studied:
                                    Kinetics
     Note(s):
                                   Handbook
     Reference(s):
     1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933
Reaction:
RX
     Reaction ID:
                                    6674984
     Reactant BRN:
                                    1238185, 1236613
     Reactant:
                                    oxygen, benzophenone, isopropylbenzene
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
                                    2
Reaction Details:
     Reaction RID:
                                    6674984.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    100 Cel
     Subject Studied:
                                    Kinetics
     Note(s):
                                   Handbook
     Reference(s):
     1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933
RX
                                    6674984.2
     Reaction RID:
     Reaction Classification:
                                   Chemical behaviour
     Temperature:
                                    15 Cel
     Subject Studied:
                                   Kinetics
    Note(s):
                                   Handbook
    Reference(s):
     1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933
```

```
Reaction:
RX
     Reaction ID:
                                    6674983
     Reactant BRN:
                                    1236613
     Reactant:
                                    oxygen, isopropylbenzene
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
    Reaction RID:
                                    6674983.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    90 Cel
     Subject Studied:
                                    Kinetics
     Note(s):
                                    Handbook
     Reference(s):
     1. Kucher et al., Kolloidn.Zh., CODEN: KOZHAG, 21, <1959>, 309; engl.
        Ausg. S. 295
RX
     Reaction RID:
                                    6674983.2
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    60 - 120 Cel
                                    20 - 60 Torr
     Pressure:
     Subject Studied:
                                   Kinetics
     Note(s):
                                   Handbook
     Pressure:
                                    60 Torr
     Reference(s):
     1. Takahashi, Kogyo Kagaku Zasshi, CODEN: KGKZA7, 57, <1954>, 363,
        Chem.Abstr., <1955>, 15789
RX
     Reaction RID:
                                    6674983.3
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    100 Cel
     Subject Studied:
                                    Kinetics
     Note(s):
                                   Handbook
     Reference(s):
     1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933
RX
     Reaction RID:
                                   6674983.4
     Reaction Classification:
                                   Chemical behaviour
     Temperature:
                                    100 - 140 Cel
     Subject Studied:
                                   Kinetics
     Note(s):
                                   Handbook
     Reference(s):
     1. Tsunoda; Matsumoto, Tokai technol. J. Japan, 17(1), <1956>, 17
RX
     Reaction RID:
                                   6674983.5
     Reaction Classification:
                                   Chemical behaviour
     Temperature:
                                   120 Cel
     Subject Studied:
                                   Kinetics
     Note(s):
                                   Handbook
     Reference(s):

    De Boer et al., Proc.K.Ned.Akad.Wet.Ser.B:Phys.Sci., CODEN: KNWBAA, <B>

        61, <1958>, 170
RX
     Reaction RID:
                                   6674983.6
     Reaction Classification:
                                   Chemical behaviour
     Other Conditions:
                                   UV-Licht
     Note(s):
                                   Handbook
     Reference(s):
     1. Hock; Lang, Chem.Ber., CODEN: CHBEAM, 77/79, <1944/1946>, 257, 261
```

Reaction:

```
RX
     Reaction ID:
                                    5093407
     Reactant BRN:
                                    1910303, 1923953
     Reactant:
                                    (1-methyl-1-phenyl-ethyl)-peroxyl,
                                    Tris-(trimethylsilyl)-silan
     Product BRN:
                                    1908117, 2040481
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
                                    Tris-(trimethyl)-silyl
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    5093407.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    72.5 Cel
     Other Conditions:
                                    also with Bu3SnH
     Subject Studied:
                                    Rate constant
     Reference(s):
     1. Chatgilialoglu, Chryssostomos; Timokhin, Vitaliy I.; Zaborovskiy,
        Andriy B.; Lutsyk, Daria S.; Prystansky, Ruslan E., Chem. Commun.,
        CODEN: CHCOFS(5), <1999>, 405 - 406; BABS-6163466
Reaction:
RX
     Reaction ID:
                                    5045464
     Reactant BRN:
                                    969405
     Reactant:
                                    isopropenylbenzene
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    5045464.1
     Reaction Classification:
                                    Preparation
     Yield:
                                    72 percent (BRN=1908117)
     Reagent:
                                    O2, Et3SiH
     Catalyst:
                                    Co(II) (tdcpp)
     Solvent:
                                    CH2Cl2, propan-2-ol
     Time:
                                    1 hour(s)
     Temperature:
                                    28 Cel
     Pressure:
                                    760 Torr
     Reference(s):
     1. Sugamoto, Kazuhiro; Matsushita, Yoh-ichi; Matsui, Takanao,
        J.Chem.Soc.Perkin Trans.1, CODEN: JCPRB4(23), <1998>, 3989-3998;
        BABS-6130087
Reaction:
RX
     Reaction ID:
                                    4495179
     Reactant BRN:
                                    7494642
     Reactant:
                                    C9H12*O3
     Product BRN:
                                    5508788, 1908117, 1905012, 605842
     Product:
                                    cumyl hydrotrioxide, 1-methyl-1-phenyl-ethyl
                                    hydroperoxide, 2-phenyl-propan-2-ol,
                                    1-phenyl-ethanone
     No. of Reaction Details:
Reaction Details:
     Reaction RID:
                                    4495179.1
     Reaction Classification:
                                    Chemical behaviour
                                    cumene
     Reagent:
     Solvent:
                                    CH2Cl2
```

Temperature: -30 Cel Other Conditions: other temperatures; activation parameters A', A0, .delta.S0<*>, A1; decomposition of ozone complexes with arenes; spectrophotometric study of kinetic regularities; possible mechanism of conversion of ozone complexes Subject Studied: Rate constant, Thermodynamic data, Kinetics Reference(s): 1. Avzyanova, E. V.; Kabal'nova, N. N.; Shereshovets, V. V., Russ.Chem.Bl., CODEN: RCBUEY, 45(2), <1996>, 356-359, Izv.Akad.Nauk Ser.Khim., CODEN: IASKEA(2), <1996>, 371-374; BABS-6013599 Reaction: Reaction ID: 4476259 Reactant BRN: 393006, 1098229, 3610848 Reactant: 2,3,5,6-tetrachloro-<1,4>benzoquinone, methanol, 4-methoxybicumene Product BRN: 6977835, 1905012, 1908117, 1859781, 3604540 Product: 2,3,5,6-tetrachloro-4-(1-methyl-1-phenylethoxy)-phenol, 2-phenyl-propan-2-ol, 1-methyl-1-phenyl-ethyl hydroperoxide, methyl-(1-methyl-1-phenyl-ethyl)-ether, 2-methoxy-2-(4'-methoxyphenyl)propane No. of Reaction Details: Reaction Details: Reaction RID: 4476259.1 Reaction Classification: Chemical behaviour Yield: 7 percent Spectr. (BRN=6977835), 7 percent Spectr. (BRN=1905012), 41 percent Spectr. (BRN=1908117), 14 percent Spectr. (BRN=1859781), 71 percent Spectr. (BRN=3604540) Reagent: 02 Solvent: tetrahydrofuran-d8 Other Conditions: Ambient temperature, Irradiation, electron transfer and fragmentation reactions of photogenerated methoxybicumene radical cations; effect of oxygen; back electron transfer in triplet ion pairs; formation of charge-transfer complexes between quinones and methoxybicumenes Subject Studied: Quantum yield, Rate constant, Product distribution Reference(s): 1. Maslak, Przemyslaw; Chapman, William H., J.Org.Chem., CODEN: JOCEAH, 61(8), <1996>, 2647-2656; BABS-6013063 Reaction: Reaction ID: 4344720 Reactant BRN: Reactant: peroxybenzoic acid-(1-methyl-1-phenyl-ethyl ester) Product BRN: 1908117 Product: 1-methyl-1-phenyl-ethyl hydroperoxide

Reaction Details:

RX

RX

Reaction RID:

No. of Reaction Details:

4344720.1

```
Reaction Classification:
                                    Preparation
     Reagent:
                                    aq. LiOH
     Solvent:
                                    tetrahydrofuran
     Reference(s):
     1. Caldwell, Sarah E.; Porter, Ned. A., J.Amer.Chem.Soc., CODEN: JACSAT,
        117(33), <1995>, 8676-8677; BABS-6002112
Reaction:
RX
     Reaction ID:
                                    3117018
     Reactant BRN:
                                    5508788
     Reactant:
                                    cumyl hydrotrioxide
                                    1236613, 1905012, 1908117, 605842
     Product BRN:
                                    isopropylbenzene, 2-phenyl-propan-2-ol,
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
                                    1-phenyl-ethanone
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    3117018.1
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                    2,6-di-tert-butyl-4-methylphenol
     Solvent:
                                    acetone-d6
     Temperature:
                                    -18 Cel
     Other Conditions:
                                   Arrhenius parameters; other temperatures,
                                    reagents ratio
     Subject Studied:
                                   Rate constant, Thermodynamic data, Mechanism
     Reference(s):
     1. Pryor, William A.; Ohto, Norio; Church, Daniel F., J.Amer.Chem.Soc.,
        CODEN: JACSAT, 104(21), <1982>, 5813-5814; BABS-5693890
Reaction:
RX
     Reaction ID:
                                   3090813
     Reactant BRN:
                                    5430954
     Reactant:
                                    <1-(1-methoxy-1-methyl-ethylperoxy)-1-methyl-
                                    ethyl>-benzene
     Product BRN:
                                   1908117
     Product:
                                   1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
     Reaction RID:
                                   3090813.1
     Reaction Classification:
                                   Preparation
     Reagent:
                                   AcOH, H2O
     Solvent:
                                   tetrahydrofuran
     Time:
                                    24 hour(s)
     Note(s):
                                   Yield given
     Reference(s):
     1. Bloodworth, A. J.; Cooksey, Christhopher J.; Korkodilos, Despoina,
        J.Chem.Soc.Chem.Commun., CODEN: JCCCAT(13), <1992>, 926-927;
       BABS-5656223
Reaction:
RX
     Reaction ID:
                                   2297353
     Reactant BRN:
                                   3610848
     Reactant:
                                   4-methoxybicumene
     Product BRN:
                                   3604540, 1908117, 1905012
     Product:
                                   2-methoxy-2-(4'-methoxyphenyl)propane,
                                   1-methyl-1-phenyl-ethyl hydroperoxide,
                                   2-phenyl-propan-2-ol
```

```
No. of Reaction Details:
                                    2
Reaction Details:
RX
     Reaction RID:
                                    2297353.1
     Reaction Classification:
                                    Preparation
     Yield:
                                    100 percent Spectr. (BRN=3604540), 20
                                    percent Spectr. (BRN=1908117), 78 percent
                                    Spectr (BRN=1905012)
     Reagent:
                                    1,4-dicyanobenzene, 02
                                    tetrahydrofuran, methanol
     Solvent:
                                    22 Cel
     Temperature:
                                    Irradiation
     Other Conditions:
     Reference(s):
     1. Maslak, Przemyslaw; Chapman, William H., Tetrahedron, CODEN: TETRAB,
        46(8), <1990>, 2715-2724; BABS-5511977
RX
     Reaction RID:
                                    2297353.2
     Reaction Classification:
                                    Preparation
     Yield:
                                    100 percent Spectr. (BRN=3604540), 78
                                    percent Spectr. (BRN=1905012), 20 percent
                                    Spectr (BRN=1908117)
                                    1,4-dicyanobenzene, 02
     Reagent:
     Solvent:
                                    tetrahydrofuran, methanol
     Temperature:
                                    22 Cel
     Other Conditions:
                                    Irradiation
     Reference(s):
     1. Maslak, Przemyslaw; Chapman, William H., Tetrahedron, CODEN: TETRAB,
        46(8), <1990>, 2715-2724; BABS-5511977
Reaction:
RX
     Reaction ID:
                                    2297352
     Reactant BRN:
                                    3610848
     Reactant:
                                    4-methoxybicumene
     Product BRN:
                                    1908117, 1905012
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
     Product:
                                    2-phenyl-propan-2-ol
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    2297352.1
     Reaction Classification:
                                    Preparation
     Reagent:
                                    oxygen
     Other Conditions:
                                    Irradiation
     Reference(s):
     1. Maslak, Przemyslaw; Chapman, Jr. William H., J.Chem.Soc.Chem.Commun.,
        CODEN: JCCCAT(23), <1989>, 1809-1811; BABS-5918901
     2. Maslak, Przemyslaw; Chapman, Jr. William H., J.Chem.Soc.Chem.Commun.,
        CODEN: JCCCAT(23), <1989>, 1809-1811; BABS-5918901
Reaction:
RX
     Reaction ID:
                                    2020496
     Reactant BRN:
                                    1910303
     Reactant:
                                    (1-methyl-1-phenyl-ethyl)-peroxyl
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
```

2020496.1

Reaction RID:

```
Reaction Classification:
                                   Chemical behaviour
                                    tBuSi(H)Me2
     Reagent:
                                    72.35 Cel
     Temperature:
     Subject Studied:
                                   Kinetics
                                   Reduction
     Reaction Type:
     Prototype Reaction:
                                   Further Variations:, Reagents
     Reference(s):
     1. Chatgilialoglu, Chryssostomos; Timokhin, Vitaliy I.; Zaborovskiy,
        Andriy B.; Lutsyk, Daria S.; Prystansky, Ruslan E., J.Chem.Soc.Perkin
        Trans.2, CODEN: JCPKBH(3), <2000>, 577 - 582; BABS-6238109
RX
     Reaction RID:
                                    2020496.2
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                   diphenylamine, O2, AIBN
     Solvent:
                                   chlorobenzene
                                   348.5 Cel
     Temperature:
     Subject Studied:
                                   Rate constant
     Reference(s):
     1. Varlamov, V. T.; Denisov, E. T., Bull.Acad.Sci.USSR
        Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 36(8), <1987>, 1607-1612,
        Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(8), <1987>, 1738-1743;
        BABS-5740678
RX
     Reaction RID:
                                    2020496.3
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
                                    <meso-tetrakis(2,6-dimethyl-3-</pre>
                                    sulfonatophenyl) porphinato>manganese(III)
                                   hydrate, NaNO3, buffer pH 10 (HCO3-/CO32-),
                                   H2O2, air
     Temperature:
                                    30 Cel
     Subject Studied:
                                   Rate constant, Equilibrium constant,
                                   Mechanism
     Reference(s):
     1. Arasasingham, Ramesh D.; Jeon, Seungwon; Bruice, Thomas C.,
        J.Amer.Chem.Soc., CODEN: JACSAT, 114(7), <1992>, 2536-2544;
        BABS-5647883
Reaction:
RX
     Reaction ID:
                                   2020495
     Reactant BRN:
                                   1910303, 2384864
     Reactant:
                                    (1-methyl-1-phenyl-ethyl)-peroxyl,
                                   hexahydroxy-<1,4>naphthoquinone
     Product BRN:
                                   1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
                                   2020495.1
     Reaction RID:
     Reaction Classification:
                                   Chemical behaviour
     Temperature:
                                   60 Cel
     Subject Studied:
                                   Rate constant
     Reference(s):
     1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,
        Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),
        <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),
        <1985>, 1471-1476; BABS-5798349
Reaction:
RX
     Reaction ID:
                                   2020494
     Reactant BRN:
                                   1910303, 2147084
     Reactant:
                                    (1-methyl-1-phenyl-ethyl)-peroxyl,
```

```
6-ethyl-2,3,5,7,8-pentahydroxy-
                                    <1,4>naphthoquinone
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
рx
     Reaction RID:
                                    2020494.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    60 Cel
     Subject Studied:
                                    Rate constant
     Reference(s):
     1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,
        Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),
        <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),
        <1985>, 1471-1476; BABS-5798349
Reaction:
РX
     Reaction ID:
                                    2020493
     Reactant BRN:
                                    1910303, 2146863
     Reactant:
                                    (1-methyl-1-phenyl-ethyl)-peroxyl,
                                    2-acetyl-3,5,6,8-tetrahydroxy-
                                    <1,4>naphthoquinone
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    2020493.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    60 Cel
     Subject Studied:
                                    Rate constant
     Reference(s):
     1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,
        Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),
        <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),
        <1985>, 1471-1476; BABS-5798349
Reaction:
RX
     Reaction ID:
                                    2020492
     Reactant BRN:
                                    1910303, 2131494
                                    (1-methyl-1-phenyl-ethyl)-peroxyl,
     Reactant:
                                    2,3,5,6,8( oder 2,5,6,7,8)-pentahydroxy-
                                    <1,4>naphthoquinone
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    2020492.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    60 Cel
     Subject Studied:
                                    Rate constant
     Reference(s):

    Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,

        Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),
        <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),
        <1985>, 1471-1476; BABS-5798349
```

```
Reaction:
     Reaction ID:
                                    2020491
     Reactant BRN:
                                    1910303, 2003780
     Reactant:
                                    (1-methyl-1-phenyl-ethyl)-peroxyl,
                                    2-acetyl-3,5,6,7,8-pentahydroxy-
                                    <1,4>naphthoquinone
     Product BRN:
                                    1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
ВX
     Reaction RID:
                                    2020491.1
     Reaction Classification:
                                    Chemical behaviour
     Temperature:
                                    60 Cel
     Subject Studied:
                                    Rate constant
     Reference(s):
     1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,
        Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),
        <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),
        <1985>, 1471-1476; BABS-5798349
Reaction:
ВX
     Reaction ID:
                                    1709985
     Reactant BRN:
                                    1236613
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    1908117, 1905012, 605842, 969616, 2056090
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
                                    2-phenyl-propan-2-ol, 1-phenyl-ethanone,
                                    phenol, bis-(1-methyl-1-phenyl-ethyl)-
                                    peroxide
     No. of Reaction Details:
                                    2
Reaction Details:
RX
                                    1709985.1
     Reaction RID:
     Reaction Classification:
                                    Chemical behaviour
     Yield:
                                    88.8 percent (BRN=1908117)
     Reagent:
                                    02, AlCl-phthalocyanine
     Time:
                                    1.1 hour(s)
     Temperature:
                                    130 Cel
     Other Conditions:
                                    mechanism; other times and temperatures;
                                    other phthalocyanine; further reagent;
                                    various concentrations of reagent;
                                    activation energies
     Subject Studied:
                                    Kinetics, Thermodynamic data, Product
                                    distribution
     Reference(s):

    Kropf, Heinz; Vogel, Werner, J.Chem.Res.Miniprint, CODEN: JRMPDM(1),

        <1986>, 0315-0342; BABS-5867413
RX
     Reaction RID:
                                    1709985.2
     Reaction Classification:
                                    Chemical behaviour
     Yield:
                                    92.8 percent (BRN=1908117)
                                    02, Sn(OH)2-phthalocyanine
    Reagent:
     Time:
                                    5.7 hour(s)
     Temperature:
                                    110 Cel
    Other Conditions:
                                   mechanism; other times and temperatures;
                                   other phthalocyanines; various
                                   concentrations of reagent; activation
                                    energies
    Subject Studied:
                                   Kinetics, Thermodynamic data, Product
```

distribution

```
Reference(s):
     1. Kropf, Heinz; Vogel, Werner; Hopf, Christiane, J.Chem.Res.Miniprint,
        CODEN: JRMPDM(1), <1986>, 0301-0314; BABS-5867412
Reaction:
RX
     Reaction ID:
                                    1709984
     Reactant BRN:
                                    1236613
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    1908117, 605842, 1905012, 969405, 969616
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
                                    1-phenyl-ethanone, 2-phenyl-propan-2-ol,
                                    isopropenylbenzene, phenol
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    1709984.1
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
     Catalyst:
                                   zinc naphthenate-1,10-phenanthroline
     Time:
                                    8 hour(s)
     Temperature:
                                   100 Cel
     Other Conditions:
                                   rate constants between 100-130 deg C
     Subject Studied:
                                   Kinetics, Product distribution
     Reference(s):
     1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR
        (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 1284-1286,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(6), <1986>, 1378-1380;
        BABS-5877997
RX
     Reaction RID:
                                   1709984.2
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
     Catalyst:
                                   1.5E-4 zinc naphthenate
     Time:
                                   3 hour(s)
                                   110 Cel
     Temperature:
     Other Conditions:
                                   activation energy; different catalyst,
                                   catalyst concentrations, reaction times and
                                   temperatures
     Subject Studied:
                                   Product distribution, Kinetics,
                                   Thermodynamic data
     Reference(s):
     1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR
        (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 122-127,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(1), <1986>, 134-139;
        BABS-5875963
Reaction:
RX
     Reaction ID:
                                   1709981
     Reactant BRN:
                                   1236613
     Reactant:
                                   isopropylbenzene
     Product BRN:
                                   605842, 1908117
     Product:
                                   1-phenyl-ethanone, 1-methyl-1-phenyl-ethyl
                                   hydroperoxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                   1709981.1
     Reaction Classification:
                                   Chemical behaviour
```

<ZnNf2>/o-phenanthroline

Catalyst:

```
6 hour(s)
     Time:
                                    110 Cel
     Temperature:
                                    dependence of the initial rate of oxidation
     Other Conditions:
                                    on the catalyst-activator ratio; effect of
                                    various catalysts; influence of the catalyst
                                    concentration on the selectivity for CHP
     Subject Studied:
                                    Product distribution
     Reference(s):
     1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR
        (Engl.Transl.), CODEN: JAPUAW, 59(5), <1986>, 1061-1063,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(5), <1986>, 1138-1140;
        BABS-5881749
Reaction:
RX
     Reaction ID:
                                    1709979
     Reactant BRN:
                                    1236613
                                    isopropylbenzene
     Reactant:
                                    1905012, 1908117, 605842, 5508788
     Product BRN:
                                    2-phenyl-propan-2-ol, 1-methyl-1-phenyl-
     Product:
                                    ethyl hydroperoxide, 1-phenyl-ethanone,
                                    cumyl hydrotrioxide
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    1709979.1
     Reaction Classification:
                                    Preparation
     Yield:
                                    2 percent (BRN=5508788)
     Reagent:
                                    ozone
     Solvent:
                                    acetone-d6
     Time:
                                    3 hour(s)
     Temperature:
                                    -40 Cel
     Note(s):
                                    Yields of byproduct given
     Reference(s):
     1. Pryor, William A.; Ohto, Norio; Church, Daniel F., J.Amer.Chem.Soc.,
        CODEN: JACSAT, 104(21), <1982>, 5813-5814; BABS-5693890
Reaction:
RX
     Reaction ID:
                                    1709978
     Reactant BRN:
                                    1236613
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    1908117, 1905012, 605842, 2056090
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide,
                                    2-phenyl-propan-2-ol, 1-phenyl-ethanone,
                                    bis-(1-methyl-1-phenyl-ethyl)-peroxide
     No. of Reaction Details:
Reaction Details:
RX
                                    1709978.1
     Reaction RID:
     Reaction Classification:
                                    Chemical behaviour
     Yield:
                                    0.36 mol (BRN=1908117), 0.035 mol
                                    (BRN=1905012), 0.0014 mol (BRN=605842),
                                    0.0015 mol (BRN=2056090)
     Reagent:
                                    2,2,3,3-tetraphenylbutane, 02
     Time:
                                    48 hour(s)
     Temperature:
                                    29.9 Cel
     Pressure:
                                    304 Torr
     Other Conditions:
                                    variation of reagent, pressure, reaction
     Subject Studied:
                                   Rate constant, Product distribution
```

Reference(s):

```
59, <1981>, 2253-2260; BABS-5663809
Reaction:
RX
     Reaction ID:
                                    1709977
                                    1236613
     Reactant BRN:
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    1905012, 1908117, 605842
     Product:
                                    2-phenyl-propan-2-ol, 1-methyl-1-phenyl-
                                    ethyl hydroperoxide, 1-phenyl-ethanone
     No. of Reaction Details:
Reaction Details:
     Reaction RID:
                                    1709977.1
     Reaction Classification:
                                    Preparation
     Yield:
                                    14 percent Spectr. (BRN=1905012), 8 percent
                                    Spectr. (BRN=1908117), 9 percent Spectr
                                    (BRN=605842)
     Reagent:
                                    dioxygen
     Catalyst:
                                    cerium (IV) ammonium nitrate,
     Solvent:
                                    acetonitrile
     Time:
                                    5 hour(s)
     Other Conditions:
                                    Ambient temperature, Irradiation
     Note(s):
                                    Title compound not separated from byproducts
     Reference(s):
     1. Baciocchi, E.; Giacco, T. Del; Sebastiani, G. V.; Rol, C., Tetrahedron
        Lett., CODEN: TELEAY, 26(28), <1985>, 3353-3356; BABS-5552479
RX
     Reaction RID:
                                    1709977.2
     Reaction Classification:
                                    Preparation
     Yield:
                                    9 percent Spectr. (BRN=605842), 8 percent
                                    Spectr. (BRN=1908117), 14 percent Spectr
                                    (BRN=1905012)
     Reagent:
                                    dioxygen
     Catalyst:
                                    cerium (IV) ammonium nitrate,
     Solvent:
                                    acetonitrile
     Time:
                                    5 hour(s)
     Other Conditions:
                                   Ambient temperature, Irradiation
     Note(s):
                                   Title compound not separated from byproducts
     Reference(s):
     1. Baciocchi, E.; Giacco, T. Del; Sebastiani, G. V.; Rol, C., Tetrahedron
        Lett., CODEN: TELEAY, 26(28), <1985>, 3353-3356; BABS-5552479
RX
     Reaction RID:
                                    1709977.3
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                    1.5E-4 M MgNf2, 6E-4 M Phen
     Catalyst:
     Time:
                                    4 hour(s)
     Temperature:
                                   110 Cel
     Other Conditions:
                                   different catalytic systems and reaction
                                    times
     Subject Studied:
                                   Product distribution
     Reference(s):

    Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR

        (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 205-207,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(1), <1986>, 217-219;
       BABS-5876061
RX
     Reaction RID:
                                   1709977.4
     Reaction Classification:
                                   Preparation
     Yield:
                                   9 percent Spectr. (BRN=605842), 14 percent
```

Spectr. (BRN=1905012), 8 percent Spectr

1. Howard, J. A.; Bennett, J. E.; Brunton, G., Can.J.Chem., CODEN: CJCHAG,

```
(BRN=1908117)
                                    dioxygen
     Reagent:
     Catalyst:
                                    cerium (IV) ammonium nitrate,
     Solvent:
                                    acetonitrile
     Time:
                                    5 hour(s)
     Other Conditions:
                                    Ambient temperature, Irradiation
                                    Title compound not separated from byproducts
     Note(s):
     Reference(s):
     1. Baciocchi, E.; Giacco, T. Del; Sebastiani, G. V.; Rol, C., Tetrahedron
        Lett., CODEN: TELEAY, 26(28), <1985>, 3353-3356; BABS-5552479
     Reaction RID:
                                    1709977.5
     Reaction Classification:
                                    Chemical behaviour
     Yield:
                                    38.0 percent (BRN=1908117), 0.28 percent
                                    (BRN=605842), 2.24 percent (BRN=1905012)
     Reagent:
     Catalyst:
                                    zinc pyrazolonate, 1,10-phenanthroline
     Time:
                                    5.0 hour(s)
     Temperature:
                                    110 Cel
     Other Conditions:
                                    effect of further monodentate and bidentate
                                    activators
     Subject Studied:
                                    Product distribution
     Reference(s):
     1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR
        (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 1287-1290,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(6), <1986>, 1381-1384;
        BABS-5877998
Reaction:
     Reaction ID:
                                    278976
     Reactant BRN:
                                   1905012
     Reactant:
                                   2-phenyl-propan-2-ol
     Product BRN:
                                   1908117
     Product:
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
Reaction Details:
     Reaction RID:
                                    278976.1
     Reaction Classification:
                                   Preparation
     Reagent:
                                   aqueous H2O2, H2SO4
     Note(s):
                                   Handbook
     Reference(s):
     1. Ross; Huettel, Chem.Ber., CODEN: CHBEAM, 89, <1956>, 2641
Reaction:
     Reaction ID:
                                   267155
     Reactant BRN:
                                   1855036
     Reactant:
                                    (.alpha.-chloro-isopropyl)-benzene
     Product BRN:
                                   1908117
     Product:
                                   1-methyl-1-phenyl-ethyl hydroperoxide
     No. of Reaction Details:
                                   1
```

Reaction Details:

RX

RX

RX

RX

RX

Reaction RID: 267155.1 Reaction Classification: Preparation

Reagent: aqueous H2O2, NaHCO3, H2SO4

Note(s): Handbook

Reference(s):

1. Ross; Huettel, Chem.Ber., CODEN: CHBEAM, 89, <1956>, 2641

```
Reaction:
RX
     Reaction ID:
                                    108026
     Reactant BRN:
                                    1236613
     Reactant:
                                    isopropylbenzene
     Product BRN:
                                    1908117
                                    1-methyl-1-phenyl-ethyl hydroperoxide
     Product:
     No. of Reaction Details:
Reaction Details:
RX
     Reaction RID:
                                    108026.1
     Reaction Classification:
                                    Preparation
     Reagent:
                                    steam, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Distillers Co. DE 819092 1949, DRP/DRBP Org.Chem.
RX
     Reaction RID:
                                    108026.2
     Reaction Classification:
                                    Preparation
                                    anthraquinone, oxygen
     Reagent:
     Other Conditions:
                                    Irradiation.UV-Belichtung
     Note(s):
                                    Handbook
     Reference(s):
     1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933, 1935
RX
     Reaction RID:
                                    108026.3
     Reaction Classification:
                                    Preparation
     Reagent:
                                    terephthalic acid, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Montecatini US 2799711 1956
RX
     Reaction RID:
                                    108026.4
                                    Preparation
     Reaction Classification:
     Reagent:
                                    acetoacetic acid ethyl ester, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Soc. Usines Chim. Rhone-Poulenc US 2674629 1953
RX
     Reaction RID:
                                    108026.5
     Reaction Classification:
                                    Preparation
     Reagent:
                                    cerium naphthenate, oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Farbenfabr. Bayer US 2655545 1951
     2. Patent: Farbenfabr. Bayer DE 889443 1951, DRP/DRBP Org.Chem.
     3. Patent: Farbenfabr. Bayer DE 969744 1950
RX
     Reaction RID:
                                    108026.6
     Reaction Classification:
                                    Preparation
     Reagent:
                                    oxygen
     Temperature:
                                    85 Cel
     Other Conditions:
                                    UV-Licht
     Note(s):
                                    Handbook
     Reference(s):
     1. George; Rideal; Robertson, Proc.R.Soc.London A, CODEN: PRLAAZ, 185,
        <1946>, 288, 292, 297
     2. Hock; Lang, Chem.Ber., CODEN: CHBEAM, 77/79, <1944/1946>, 257, 261
RX
     Reaction RID:
                                    108026.7
     Reaction Classification:
                                    Preparation
     Reagent:
                                    Na2CO3, oxygen
     Note(s):
                                    Handbook
```

```
Reference(s):
     1. Patent: Allied Chem. & Dye Corp. US 2629744 1950
     2. Patent: Allied Chem. & Dye Corp. US 2681936 1950
ВX
     Reaction RID:
                                    108026.8
     Reaction Classification:
                                    Preparation
                                    aqueous sodium stearate, oxygen
     Reagent:
                                    Handbook
     Note(s):
     Reference(s):
     1. Armstrong et al., J.Chem.Soc., CODEN: JCSOA9, <1950>, 666
     2. Patent: Hercules Powder Co. US 2547938 1947
RX
                                    108026.9
     Reaction RID:
                                    Chemical behaviour
     Reaction Classification:
     Yield:
                                    18 percent Chromat. (BRN=1908117)
     Reagent:
                                    102, 9-diazofluorene, meso-
                                    tetraphenylporphine
                                    benzene
     Solvent:
     Time:
                                    30 min
     Temperature:
                                    20 Cel
     Other Conditions:
                                    Irradiation, O-transfer reaction; trapping
                                    of carbonyl oxide from 9-diazofluorene
     Subject Studied:
                                   Product distribution, Mechanism
     Reference(s):
     1. Sawaki, Yasuhiko; Kato, Hiroshi; Ogata, Yoshiro, J.Amer.Chem.Soc.,
        CODEN: JACSAT, 103(13), <1981>, 3832-3837; BABS-5691150
RX
     Reaction RID:
                                    108026.10
     Reaction Classification:
                                    Preparation
     Reagent:
                                    oxygen
     Time:
                                    8 hour(s)
     Temperature:
                                    110 Cel
     Reference(s):
     1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR
        (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 2490-2494,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(12), <1985>, 2696-2701;
        BABS-5877528
RX
     Reaction RID:
                                    108026.11
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                   p-dihydroxybenzene, azoisobutyronitrile
     Solvent:
                                    acetic acid
     Temperature:
                                    60 Cel
     Other Conditions:
                                    other reagent, other solvent, other
                                    temperature, various concentrations of the
                                    substrate, various concentrations of the
                                    reagent
     Subject Studied:
                                   Kinetics, Rate constant
     Reference(s):

    Nikolaevskii, A.N.; Kaloerova, V.G.; Kucher, R.V., J.Org.Chem.USSR

        (Engl.Transl.), CODEN: JOCYA9, 17, <1981>, 510-514, Zh.Org.Khim.,
        CODEN: ZORKAE, <1> 17(3), <1981>, 595-600; BABS-5631011
RX
     Reaction RID:
                                   108026.12
     Reaction Classification:
                                   Preparation
     Reagent:
                                   azobisisobutyronitrile
     Time:
                                    6 hour(s)
     Temperature:
                                    95 Cel
     Reference(s):
     1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR
        (Engl.Transl.), CODEN: JAPUAW, 59(5), <1986>, 993-996,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(5), <1986>, 1072-1076;
       BABS-5881743
```

```
Reaction Classification:
                                    Preparation
     Reagent:
                                    oxygen
     Note(s):
                                    Handbook
     Reference(s):
     1. Patent: Shell Devel. Co. US 2633476 1952
RX
     Reaction RID:
                                    108026.14
     Reaction Classification:
                                    Chemical behaviour
                                    O2, diethyl ester of 2-chloro-2(1-
     Reagent:
                                    cyclohexenyl)ethylenylphosphonic acid, AIBN
     Temperature:
                                    59.9 Cel
     Other Conditions:
                                    antioxidant effect of further dialkyl esters
                                    and dialkyl thioesters of
                                    2-chloro-2(1-cyclohexenyl)ethylenylphosphoni
                                    c acid at various temperature; effect of O2
                                    partial pressure on the initiated oxidation
     Subject Studied:
                                    Mechanism
     Reference(s):
     1. Ivanov, Slavi K.; Shopova, Nicolaida St.; Angelov, Christo M.,
        Phosphorus Sulfur, CODEN: PREEDF, 26, <1986>, 105-110; BABS-5827359
RX
     Reaction RID:
                                    108026.15
     Reaction Classification:
                                    Preparation
     Reagent:
                                    02, azobisisobutyronitrile
     Catalyst:
                                    monophenanthrolinezinc(II) pyrazolonate
     Temperature:
                                    75 Cel
                                    760 Torr
     Pressure:
     Reference(s):
     1. Kozlov, S. K.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN:
        JAPUAW, 59(7), <1986>, 1519-1521, Zh.Prikl.Khim.(Leningrad), CODEN:
        ZPKHAB, 59(7), <1986>, 1633-1635; BABS-5883617
RX
     Reaction RID:
                                    108026.16
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                    02, 2-cyano-2-propyl hydroperoxide
     Temperature:
                                    90 Cel
     Other Conditions:
                                    further oxidation initiators, further
                                    temperatures
     Subject Studied:
                                    Kinetics
     Reference(s):
     1. Burghardt, Aleksandra; Kulicki, Zdzislaw, Monatsh.Chem., CODEN: MOCMB7,
        115, <1984>, 87-92; BABS-5796729
RX
     Reaction RID:
                                    108026.17
     Reaction Classification:
                                   Preparation
     Reagent:
                                   02, 2-cyano-2-propyl hydroperoxide
     Reference(s):
     1. Burghardt, Aleksandra; Kulicki, Zdzislaw, Monatsh.Chem., CODEN: MOCMB7,
        115, <1984>, 87-92; BABS-5796729
RX
     Reaction RID:
                                    108026.18
     Reaction Classification:
                                    Chemical behaviour
     Reagent:
                                   O2, AIBN
     Temperature:
                                    60 Cel
     Other Conditions:
                                   further reagents, initiation rates, kinetic
                                    curves
     Reference(s):
     1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,
        Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),
        <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),
        <1985>, 1471-1476; BABS-5798349
ВX
     Reaction RID:
                                   108026.19
```

108026.13

Reaction RID:

```
Reagent:
     Catalyst:
                                   copper(I) and copper(II) compounds
     Temperature:
     Other Conditions:
                                   var. pressure O2, also pyridine as reagent
     Subject Studied:
                                   Mechanism
     Reference(s):
     1. Stec, Zbigniew; Kulicki, Zdzislaw, Pol.J.Chem., CODEN: PJCHDQ, 57(7-9),
        <1983>, 941-945; BABS-5804264
RX
                                    108026.20
     Reaction RID:
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
                                   oxygen
                                   CdNf2
     Catalyst:
     Time:
                                    8 hour(s)
     Temperature:
                                   110 Cel
     Other Conditions:
                                   var. catalyst
     Subject Studied:
                                   Kinetics
     Reference(s):
     1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR
        (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 2490-2494,
        Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(12), <1985>, 2696-2701;
        BABS-5877528
RX
     Reaction RID:
                                   108026.21
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
                                   02, azobisisobutyronitrile
     Catalyst:
                                   monophenanthrolinezinc(II) pyrazolonate
     Temperature:
                                   60 - 85 Cel
                                   760 Torr
     Pressure:
     Other Conditions:
                                   further pressures, catalyst
     Subject Studied:
                                   Mechanism, Thermodynamic data, Kinetics
     Reference(s):
     1. Kozlov, S. K.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN:
        JAPUAW, 59(7), <1986>, 1519-1521, Zh.Prikl.Khim.(Leningrad), CODEN:
        ZPKHAB, 59(7), <1986>, 1633-1635; BABS-5883617
RX
     Reaction RID:
                                   108026.22
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
                                   02
     Catalyst:
                                   Co(acac)2
     Time:
                                   10 hour(s)
     Temperature:
                                   60 Cel
     Other Conditions:
                                   with crown ethers; rate of oxidation
     Subject Studied:
                                   Product distribution
     Reference(s):
     1. Kochinashvili, M. V.; Kuramshin, E. M.; Kotlyar, S. A.; Zlot-skii, S.
        S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN:
        JAPUAW, 62(7.2), <1989>, 1562-1564, Zh.Prikl.Khim.(Leningrad), CODEN:
        ZPKHAB, 62(7), <1989>, 1681-1684; BABS-5512252
RX
     Reaction RID:
                                   108026.23
     Reaction Classification:
                                   Preparation
     Reagent:
                                   NaCl, KNO3, oxygen
     Note(s):
                                   Handbook
     Reference(s):
     1. Patent: Allied Chem. & Dye Corp. US 2776999 1952
RX
     Reaction RID:
                                   108026.24
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
     Catalyst:
                                   different cobalt catalysts
     Subject Studied:
                                   Kinetics
     Reference(s):
```

Chemical behaviour

Reaction Classification:

```
Collect.Czech.Chem.Commun., CODEN: CCCCAK, 51(9), <1986>, 1958-1963;
        BABS-5561803
RX
     Reaction RID:
                                    108026.25
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
                                   dioxygen, cumene hydroperoxide,
                                    2,4-pentanedionates of Cr(III)
     Solvent:
                                   heptane
     Temperature:
                                    60 Cel
     Other Conditions:
                                    other radical initiator and
                                    2,4-pentanedionates of 3d-transition metals,
                                   various concentration of the reagents
     Reference(s):
     1. Lunak, Stanislav; Chmelikova, Ruzena; Lederer, Pavel,
        Collect.Czech.Chem.Commun., CODEN: CCCCAK, 56(2), <1991>, 344-350;
        BABS-5535278
RX
     Reaction RID:
                                    108026.26
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
                                   1,4,7,10,13,16-hexaoxacyclooctadecane
     Temperature:
     Other Conditions:
                                   oxidation
     Subject Studied:
                                   Rate constant
     Reference(s):
     1. Kochinashvili, M. V.; Kuramshin, E. M.; Zlot-skii, S. S.; Rakhmankulov,
        D. L., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 60(3.2), <1990>,
        574-577, Zh.Obshch.Khim., CODEN: ZOKHA4, 60(3), <1990>, 657-660;
        BABS-5537965
RX
     Reaction RID:
                                   108026.27
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
     Catalyst:
                                   phenanthroline-pyrazolone-Zn(II)-complex
     Temperature:
                                   110 Cel
     Other Conditions:
                                   other temperature, other catalysts,
                                   additives
     Subject Studied:
                                   Kinetics
     Reference(s):

    Kozlov, S. K., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 60(1.2),

        <1990>, 153-157, Zh.Obshch.Khim., CODEN: ZOKHA4, 60(1), <1990>,
        175-180; BABS-5531529
RX
     Reaction RID:
                                   108026.28
     Reaction Classification:
                                   Chemical behaviour
     Reagent:
                                   MeOCH2CH(SH)CH2NH(m-MePh), air,
                                   azoisobutyronitrile
     Solvent:
                                   chlorobenzene
     Temperature:
                                   110 Cel
     Other Conditions:
                                   var. methoxy-substituted
                                   1,2-aminopropanethiols
     Subject Studied:
                                   Mechanism, Rate constant
     Reference(s):
     1. Farzaliyev, V. M.; Allakhverdiyev, M. A.; Rzayeva, I. A.; Akhundova, M.
       M.; Nasirova, F. N.; Guseinova, A. T., Pet.Chem.USSR (Engl.Transl.),
       CODEN: PECHAM, 34(6), <1994>, 524-529, Neftekhimiya, CODEN: NEFTAH,
        34(6), <1994>, 537-541; BABS-5971722
RX
     Reaction RID:
                                   108026.29
    Reaction Classification:
                                   Chemical behaviour
    Reagent:
                                   oxygen
     Catalyst:
                                   tetraethylammonium perchlorate
    Solvent:
                                   chlorobenzene, benzonitrile
     Time:
                                   210 min
```

1. Setinek, Karel; Drapakova, Stanislava; Prokop, Zdenek,

```
Kinetics
     Subject Studied:
     Reaction Type:
                                     Oxidation
     Prototype Reaction:
                                     Further Variations:, Catalysts
     Reference(s):
     1. Opeida, I. A.; Zalevskaya, N. M., Russ. J. Org. Chem., CODEN: RJOCEQ,
        32(4), <1996>, 524 - 529, Zh.Org.Khim., CODEN: ZORKAE, 32(4), <1996>,
        545 - 550; BABS-6148286
RX
     Reaction RID:
                                     108026.30
     Reaction Classification:
                                     Chemical behaviour
     Reagent:
                                     02, aq. sodium laurate
     Temperature:
                                     75 Cel
                                     750.06 Torr
     Pressure:
     Other Conditions:
                                     rate of emulsion oxidation; other sodium
                                     alkylcarboxylaates, var. organic solvents,
                                     var. pH
     Subject Studied:
                                     Mechanism
     Reference(s):

    Panicheva, L. P.; Turnaeva, E. A.; Panichev, S. A.; Yuffa, A. Ya.,
Pet.Chem.USSR (Engl.Transl.), CODEN: PECHAM, 38(3), <1998>, 164 - 169,

        Neftekhimiya, CODEN: NEFTAH, 338, <1998>, 179 - 184; BABS-6172166
RX
     Reaction RID:
                                     108026.31
     Reaction Classification:
                                     Preparation
     Reagent:
                                     NaCl, BaSO4, oxygen
     Note(s):
                                     Handbook
     Reference(s):
     1. Patent: Allied Chem. & Dye Corp. US 2776999 1952
RX
     Reaction RID:
                                     108026.32
     Reaction Classification:
                                     Preparation
     Reagent:
                                     aqueous NaOH, oxygen
     Note(s):
                                     Handbook
     Reference(s):
     1. Patent: Hercules Powder Co. US 2619510 1951
     2. Patent: Hercules Powder Co. US 2663740 1952
     3. Patent: Hercules Powder Co. US 2548435 1946
     4. Patent: Hercules Powder Co. US 2632772 1948
     5. Patent: Distillers Co. DE 926426 1949, DRP/DRBP Org.Chem.
RX
     Reaction RID:
                                     108026.33
     Reaction Classification:
                                     Preparation
     Reagent:
                                     aqueous NaOH, ozone, oxygen
     Note(s):
                                     Handbook
     Reference(s):
     1. Patent: Bergwerksges. Hibernia US 2827493 1952
RX
     Reaction RID:
                                     108026.34
     Reaction Classification:
                                     Preparation
     Reagent:
                                     NaHCO3, oxygen
     Note(s):
                                     Handbook
     Reference(s):
     1. Patent: Allied Chem. & Dye Corp. US 2577768 1949
RX
     Reaction RID:
                                     108026.35
     Reaction Classification:
                                     Preparation
     Reagent:
                                     Ca(OH)2, oxygen
     Note(s):
                                     Handbook
     Reference(s):
     1. Patent: Hercules Powder Co. US 2632774 1949
RX
     Reaction RID:
                                     108026.36
```

Preparation

84.85 Cel

Temperature:

Reaction Classification:

Reagent: CaCO3, oxygen

Note(s): Handbook

Reference(s):

Patent: Allied Chem. & Cye Corp. US 2613227 1950
 Patent: Allied Chem. & Cye Corp. DE 864398 1951

Reaction:

RX

Reaction ID: 51759

Reactant BRN: 1236613, 1098229

Reactant: isopropylbenzene, methanol

Product BRN: 1908117

Product: 1-methyl-1-phenyl-ethyl hydroperoxide

No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 51759.1
Reaction Classification: Preparation
Reagent: oxygen
Note(s): Handbook

Reference(s):

1. Patent: Montecatini US 2843633 1954

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 6 Sep 2002 VOL 137 ISS 11 FILE LAST UPDATED: 5 Sep 2002 (20020905/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

```
=> s 13 and (water or h2o or aqueous)
          4694 L3
       1940644 WATER
        212526 WATERS
       1991299 WATER
                  (WATER OR WATERS)
        918320 H2O
        147657 AQUEOUS
             1 AQUEOUSES
        147658 AQUEOUS
                  (AQUEOUS OR AQUEOUSES)
        926014 AO
           118 AOS
        926086 AQ
                  (AQ OR AQS)
        961992 AQUEOUS
                  (AOUEOUS OR AO)
L4
           819 L3 AND (WATER OR H2O OR AQUEOUS)
=> s 14 and (mixture or composition)
         60967 MIXTURE
        118399 MIXTURES
        176682 MIXTURE
                  (MIXTURE OR MIXTURES)
       1323492 MIXT
        458147 MIXTS
       1620917 MIXT
                  (MIXT OR MIXTS)
       1667750 MIXTURE
                  (MIXTURE OR MIXT)
        592411 COMPOSITION
        239065 COMPOSITIONS
        827686 COMPOSITION
                  (COMPOSITION OR COMPOSITIONS)
       1164582 COMPN
        456556 COMPNS
       1419992 COMPN
                  (COMPN OR COMPNS)
       1853040 COMPOSITION
                  (COMPOSITION OR COMPN)
L5
           375 L4 AND (MIXTURE OR COMPOSITION)
```

```
=> s l1
```

L11

18 L1

=> d ide

L11 ANSWER 1 OF 18 CHEMCATS COPYRIGHT 2002 ACS

Accession No. (AN): 2002:1282035 CHEMCATS

Catalog Name (CO): Acros Organics Publication Date (PD): 16 Apr 2002

(ON): 34996 Order Number

Chemical Name (CN): Cumyl hydroperoxide

(CN): Cumolhydroperoxid; Cumene hydroperoxide; Synonym

Isopropylbenzolhydroperoxid;

Isopropylbenzolhydroperoxid; Cumene hydroperoxide

CAS Registry No. (RN): 80-15-9

Structure

=> d all

L11 ANSWER 1 OF 18 CHEMCATS COPYRIGHT 2002 ACS

Accession No. (AN): 2002:1282035 CHEMCATS

Catalog Name (CO): Acros Organics (PD): 16 Apr 2002 (ON): 34996 Publication Date

Order Number

Chemical Name (CN): Cumyl hydroperoxide

Synonym (CN): Cumolhydroperoxid; Cumene hydroperoxide;

Isopropylbenzolhydroperoxid;

Isopropylbenzolhydroperoxid; Cumene hydroperoxide

CAS Registry No. (RN): 80-15-9

Purity : 80%

Structure :

PROPERTIES

Density : 1.06 Melting Point : -30 C Flash Point : 83.00

REGULATORY INVENTORIES

TSCA : Y

EINECS : 201-254-7

REFERENCES

RTECS : MX2450000

PRICES

Quantity : 5.00 G, Price: \$8.90 Quantity : 250.00 G, Price: \$27.00

COMPANY INFORMATION

Acros Organics Janssens Parmaceuticalaan 3A Geel, 2440 Belgium

Phone: +32 14 57 52 11 Fax: +32 14 59 34 34 Web: http://www.acros.be Email: info@acros.com

FISHER SCIENTIFIC USA 2000 Park Lane Drive Pittsburgh, PA, 15275-1126 USA

Tel.: 1-800-766-7000 Telefax: 1-800-926-1166

FISHER SCIENTIFIC 1 Reagent Lane Fair Lawn, NJ, 07410 USA

Tel.: 1-201.703.3163 Fax: 1-201.703.3105

RESCO TRADE Hoveniersstraat 34 A Kortrijk, 8500 Belgium

Tel.: +32 56 260 260
Telefax: +32 56 260 270
Telex: 85204 rtrade
Filter Service NV/SA
Handelsstrasse 16,
4700 Eupen Belgium
Tel.:+32 87 59 51 70
Telefax: +32 87 59 51 79

KEM-en-TEC A/S Lers Parkall 42 Copenhagen, DK-2100 Denmark

Tel.: (**45)39 27 17 77 Fax: (**45)39 20 01 78

UNITED SCIENTIFIC EQUIPMENT CO. 49, Demeschk Street El-Mohandessin, Giza Egypt

Tel.: (**20)2.361.4216 Fax: (**20)2.361.3211 BIO-ART Pepleri St. 12-23 Tartu, EE-2400 Estonia

Tel.: 003727434067 Fax: 003727434067

TAMRO CORPORATION P O BOX 11 Rajatorpantie 41B Fin, Vantaa, 01641 Finland

Tel.: +358204454711 Fax: +35804454717

ADVANCED TECHNOLOGY & INDUSTRIAL CO. 8/F, Blk H, Kingland Building 739 Nathan Road Mongkog, Kowloon Hong-Kong People's Republic of China

Tel.: (**852)2390.2293 Fax: (**852)2789.8314

NEBOTRADE 1394 Budapest Pf.: 360 Budapest Hungary

Tel.: **361 214 5000 Fax: **361 214 5000

1977:600365 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 87:200365

Study of intermolecular interactions in the TITLE:

cumene hydroperoxide-water

system by the proton magnetic resonance method

Markaryan, Sh. A.; Beileryan, N. M.; Grigoryan, S. K. AUTHOR (S):

Erevan. Gos. Univ., Yerevan, USSR CORPORATE SOURCE: SOURCE:

Zh. Fiz. Khim. (1977), 51(9), 2385-7

CODEN: ZFKHA9

DOCUMENT TYPE: Journal LANGUAGE: Russian

AΒ NMR data indicated that in the title system proton exchange occurs between PhCMe200H (I) and H2O. At 97:3 I-H2O the rate const. for this exchange is 85 s-1. Interactions between the .pi. system of I and H2O also occur.

Protonation and Proton transfer reaction IT (in cumene hydroperoxide-water system)

ΙT Nuclear magnetic resonance

(proton exchange in cumene hydroperoxide-

water system in relation to)

7732-18-5, properties IT RL: PRP (Properties)

(interaction of, with cumene hydroperoxide)

ΙT 80-15-9

RL: PRP (Properties)

(interaction of, with water)

ACCESSION NUMBER: 1977:600365 CAPLUS

DOCUMENT NUMBER: 87:200365

Study of intermolecular interactions in the TITLE:

cumene hydroperoxide-water

system by the proton magnetic resonance method

AUTHOR(S):

Markaryan, Sh. A.; Beileryan, N. M.; Grigoryan, S. K.

CORPORATE SOURCE: Erevan. Gos. Univ., Yerevan, USSR Zh. Fiz. Khim. (1977), 51(9), 2385-7 SOURCE:

CODEN: ZFKHA9

DOCUMENT TYPE: Journal LANGUAGE: Russian

NMR data indicated that in the title system proton exchange occurs between PhCMe2OOH (I) and H2O. At 97:3 I-H2O the rate const. for this exchange is 85 s-1. Interactions between the .pi. system of I and H2O also occur.

Protonation and Proton transfer reaction IT (in cumene hydroperoxide-water system)

IT Nuclear magnetic resonance

(proton exchange in cumene hydroperoxide-

water system in relation to)

7732-18-5, properties ΙT RL: PRP (Properties)

(interaction of, with cumene hydroperoxide)

IT 80-15-9

RL: PRP (Properties)

(interaction of, with water)

```
7227471 1%
                (1)
          256 L5 AND 1%
L6
=> s 15 and weight percent
        87980 WEIGHT
         7556 WEIGHTS
         93412 WEIGHT
               (WEIGHT OR WEIGHTS)
       1272798 WT
        94569 WTS
       1321675 WT
                (WT OR WTS)
       1348263 WEIGHT
                (WEIGHT OR WT)
         67936 PERCENT
         1270 PERCENTS
         69001 PERCENT
                (PERCENT OR PERCENTS)
          2940 WEIGHT PERCENT
               (WEIGHT (W) PERCENT)
            0 L5 AND WEIGHT PERCENT
L7
=> s 15 and percent water
         67936 PERCENT
         1270 PERCENTS
         69001 PERCENT
                (PERCENT OR PERCENTS)
       1940644 WATER
       212526 WATERS
       1991299 WATER
                (WATER OR WATERS)
          233 PERCENT WATER
                (PERCENT (W) WATER)
L8
            0 L5 AND PERCENT WATER
=> s 15 and % water
      1940644 WATER
       212526 WATERS
      1991299 % WATER
                (WATER OR WATERS)
L9
          209 L5 AND % WATER
=> d 200-209 ibib abs
   ANSWER 200 OF 209 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1968:22368 CAPLUS
DOCUMENT NUMBER:
                       68:22368
TITLE:
                       Copolymer of vinyl acetate and acrylamide
INVENTOR(S):
                       Lanthier, Raymond
PATENT ASSIGNEE(S):
                       Shawinigan Chemicals Ltd.
SOURCE:
                        Brit., 10 pp.
                        CODEN: BRXXAA
DOCUMENT TYPE:
                       Patent
LANGUAGE:
                       English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
    PATENT NO. KIND DATE
                                        APPLICATION NO. DATE
     -----
GB 1092030 19671122 PRIORITY APPLN. INFO.:
                                      CA
                                                          19651015
```

AB A process for prepg. aq. emulsions of a random copolymer of

=> s 15 and 1%

vinyl acetate (I) and acrylamide (II) contg. 6-15% II is described. Specific proportions of the monomers are copolymd. in an aq. medium with a redox catalyst system at a suitable pH (5-7) in a suitable temp. range (40-5.degree.) and with addn. of the ingredients to the polymn. medium in a manner that precluded undesired homopolymn. of either monomer. Thus, 30 g. I contg. 0.5 ml. tert-BuOOH (III) was added to a mixt. of water 250, II 10, and Gafac PE-510 (a polyoxyethylenated phosphate anionic surfactant) 1 g. The mixt. was agitated while a stream of N was introduced and heated to 40.degree.. ' Three solns. of 2 g. NaHSO3 and 2 g. Na2HPO4 in 50 ml. H2O, 30 g. II in 70 ml. water, and 1.5 ml. III in 348 g. I were added simultaneously over a period of 3 hrs. After cooling to room temp. and filtering through a stainless steel screen having 0.25-mm. openings, a smooth, creamy, stable emulsion contg. 54.02% solids was obtained. The I-II copolymer contained 10.6% II by wt. of the I in the copolymer. had superior strength when used as an adhesive to bond 2 blocks of hardwood.

L9 ANSWER 201 OF 209 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1967:517526 CAPLUS DOCUMENT NUMBER: 67:117526

DOCUMENT NUMBER:

Dienic monomer polymerization using alcohol-peroxide TITLE:

catalysts system

INVENTOR(S): Burke, Oliver W., Jr.; Stahly, Eldon E.

SOURCE: U.S., 4 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
US 3333015 19670725 US 19631119 PATENT NO. KIND DATE

Unsatd. liquid polymers of C4-8 conjugated diene monomers for use in the formation of protective coatings, inks, and adhesives are prepd. in the presence of an org. peroxy free radical generating catalyst in homogeneous mixt. with a C1-6 alc. Thus, butadiene 70.5, methacrylic acid 4.5, iso-PrOH 35.0, and 75% cumene hydroperoxide 4.0 parts was heated to 130.degree. while being stirred at 600 rpm. and maintained for 1.5 hrs., 25 parts styrene added, the polymn. continued for 1.5 hrs. at 130.degree., and the **mixt**. devolatilized at 140.degree./<5 mm. to give a 57% yield of water-white polymer having Brookfield viscosity 4230 poises at 30.degree. and <0.2% volatiles. Other catalysts used were tert-butyl hydroperoxide, di-tert-butyl peroxide, p-menthane hydroperoxide, and partially peroxidized tung oil. tert-BuOH and MeOH could be used in place of iso-PrOH.

ANSWER 202 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:516810 CAPLUS
DOCUMENT NUMBER: 67:116810
TITLE: Color-stabilized epoxides

INVENTOR(S): Goldsmith, William F.; Marples, David F.

PATENT ASSIGNEE(S): Union Carbide Corp.

Brit., 8 pp. SOURCE: CODEN: BRXXAA

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
GB 1074003 19670628 GB 19640 19640624 Color-stabilized epoxides contain an inhibiting amt. of a peroxide compn., which is added at 70-100.degree.C., and are used to prep. color-stabilized resins. Thus, 5 wt. % 30% aq. H2O2 was added to 1000 g. 3,4-epoxy-6-methylcyclohexylmethyl 3,4-epoxy-6-methylcyclohexanecarboxylate, the mixt. heated at 95-7.degree.C. for 3 hrs., and the water evapd. to 70-80.degree.C./1 mm. for 2 hrs. to give an epoxy compd. having Gardner color 5.5 after 1 hr. at 350.degree.F. compared to 11.5 for an unstabilized epoxide. Varying the amt. of 30% aq. H2O2 affected the color stability after 16 hrs. at 98 .+-. 2.degree. as follows (wt. % 30% aq. H2O2 and Gardner color given): 0, 5.7; 0.1, 1.2; 0.3, 1.2; 1.0, 1.2; 3.0, 3.0; 10.0, 7.0. Org. peroxides were similarly used as stabilizers.

L9 ANSWER 203 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:491513 CAPLUS

DOCUMENT NUMBER: 67:91513

TITLE: Synthetic rubbers

INVENTOR(S): Richter, Johannes; Herte, Paul; Bochmann, Dieter;

Neupert, Hans

SOURCE: Ger. (East), 4 pp.

CODEN: GEXXA8

DOCUMENT TYPE:

Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. APPLICATION NO. DATE KIND DATE ----------DD 55827 19670505 DD 19660826 Synthetic rubbers with better overall properties are prepd. from AΒ 1,3-dienes such as butadiene (I) and its mixt. with styrene (II), acrylonitrile, or other vinyl homologs in the presence of special alkylaryl hydroperoxide catalysts. Thus, a typical compn. consists of I 70, II 30, resin acid 2.25, fatty acid 2.10, Wotamol 0.10, KOH 1.18, p-diisopropylbenzene monohydroperoxide (III) 0.18, triethylenetetramine 0.02, Na3PO4 0.10, and water 150 parts. Comparison of the above compn. with controls not using III showed that the test compn. had much better vulcanization values and lower Huggins const. Other hydroperoxide catalysts used were isopropylbenzene hydroperoxide and chlorotriisopropylbenzene monohydroperoxide.

L9 ANSWER 204 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:436225 CAPLUS

DOCUMENT NUMBER: 67:36225

TITLE: Polarographic analysis of waste waters from

phenol and acetone production Shleina, T. T.; Buzlanova, M. M. Zavod. Lab. (1967), 33(3), 290-3

CODEN: ZVDLAU

DOCUMENT TYPE: Journal LANGUAGE: Russian

AUTHOR (S):

SOURCE:

The mixt. of acetophenone and mesityl oxide was reduced polarographically in 0.5N KOH medium at potentials E1/2 = -1.44 v. and E1/2 = -1.54 v. vs. Hg pool. The differential polarography and the addn. method for quant. evaluation were used. The other components of waste waters did not interfere. The relative error was .+-.4%. The mixt. of cumene hydroperoxide, H2O2, and acetophenone was reduced in 0.05N LiCl medium at potentials E1/2 = -0.3 v., E1/2 = -1.25 v., and E1/2 = -1.75 v. For quant. evaluation the calibration curves of single standard components were used, with relative error .+-.2-4%. The sensitivity was 0.01-0.09 mg./ml. The detn. of .alpha.-methylstyrene (I) was made by the Alekseeva, et al., method (Alekseeva, et al., CA 59: 5341a) after conversion of I to the pseudo-nitroso compd. which was

reduced at potential E1/2 = 0.2 v. compared with the S.C.E. The presence of PhOH >0.05 mg./ml. interfered. The relative error was .+-.3%, the sensitivity 0.03 mg.I/ml.

ANSWER 205 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:422479 CAPLUS DOCUMENT NUMBER: 67:22479

TITLE: Unsaturated polyester curing system consisting of

cumene hydroperoxide, methyl ethyl ketone peroxide,

and thioglycolic acid

Montesano, Lewis INVENTOR(S):

PATENT ASSIGNEE(S): Bell Telephone Laboratories, Inc.

U.S., 2 pp. SOURCE:

CODEN: USXXAM DOCUMENT TYPE:

Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

> PATENT NO. KIND DATE APPLICATION NO. DATE US 3318974 19670509 US -----19650323

Styrene-polyester (I) is cured with a critical mixt. of AB free-radical initiators. Thus, 100 parts I, viscosity 600-750 cp., sp. gr. 1.11-1.13, a 7:3 mixt. of a polyester from phthalic anhydride, maleic anhydride, and propylene glycol with styrene, was thoroughly mixed with cumene hydroperoxide 0.25, Me Et ketone peroxide 0.5, and thioglycolic acid (II) 0.5 part. After 5 min. at room temp. the mixt. had gelled to form a water-white hard resin without cracks. The same results were obtained with 0.25 parts II.

ANSWER 206 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:116617 CAPLUS

DOCUMENT NUMBER: 66:116617

TITLE: Polyacrylonitrile solutions for spinning

Farbenfabriken Bayer A.-G. PATENT ASSIGNEE(S):

SOURCE: Neth. Appl., 12 pp.

CODEN: NAXXAN

DOCUMENT TYPE: Patent LANGUAGE: Dutch FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ----------

NL 6608595 19661227

PRIORITY APPLN. INFO.: DE 19650623

Acrylonitrile, alone or with another ethylenic unsatd. monomer, in HCONMe2 is polymd. at 30-60.degree. in the presence of an org. peroxide and an .alpha.-hydroxy-.alpha.-aminosulfone having the formula [RSO2C(R1)R2]nX, in which R is an aliphatic or aromatic hydrocarbon radical, R1 and R2 are H atoms or alkyl radicals, n is 1 or 2, and X is OH or NR3, R3 being an alkyl, hydroxyalkyl or an aryl radical, optionally with addn. of a strong mineral acid. Thus, in a closed 100-ml. app. completely filled, the reaction mixt. consisted of 65 g. HCONMe2, 32.7 g. acrylonitrile, and 2.3 g. Me acrylate. The polymerization took place in the presence of 0.3 g. cumene hydroperoxide and 0.3 g. (ClC6H4SO2CH2)2NMe. The filled app. was kept at 45.degree. for 10 hrs. in a water bath. The relative viscosity of 0.5% polymer soln. at 20.degree. in HCONMe2 was 1.85, yield was 59%, and the soln. was pale yellow. With 0.2 g. concd. H2SO4 in addn. to the above ingredients, the yield was 51%, relative viscosity 1.94, and the soln. was colorless.

ACCESSION NUMBER: 1967:37567 CAPLUS

DOCUMENT NUMBER: 66:37567

Oxidation of sulfoxides with hydroperoxides TITLE:

Kuhnen, Ludwig AUTHOR(S):

CORPORATE SOURCE: Chem. Werke Huels A.-G., Marl, Ger. Angew. Chem. (1966), 78(20), 937 SOURCE:

CODEN: ANCEAD

DOCUMENT TYPE: Journal LANGUAGE: German

Sulfides and sulfoxides were oxidized to sulfones by equimolar amts. of org. hydroperoxides in the presence of V, Mo, or Ti compds. in almost quant. yields. The sulfides and sulfoxides, dissolved in benzene, EtOAc, or EtOH, were mixed with the catalyst and heated to 50 to 70.degree., and the org. hydroperoxide was then added slowly. The reaction was complete as soon as only traces of peroxide could be detected with KI in the reaction mixt. The sulfones were then isolated by crystn. or distn. PhSMe in benzene was oxidized with tert-butyl hydroperoxide in the presence of molybdenyl acetylacetonate to produce PhSO2Me in 98% yield. Me2SO4 was oxidized with cumyl .alpha.-hydroperoxide in the presence of V205 to give Me2SO2 in 91% yield. These reactions proceeded without the presence or formation of water or carboxylic acids.

ANSWER 208 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:19053 CAPLUS

DOCUMENT NUMBER: 66:19053

TITLE: Vinyl chloride polymers or copolymers PATENT ASSIGNEE(S): Societa Edison S.p.A.-Settore Chimico

SOURCE: Neth. Appl., 11 pp.

CODEN: NAXXAN

DOCUMENT TYPE:

Patent Dutch LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

KIND DATE PATENT NO. APPLICATION NO. DATE -----

19660823 NL 6601847

PRIORITY APPLN. INFO.: IT19650222

The polymerization or copolymerization of vinyl chloride at low temps. and in the presence of a tetravalent Ce salt and an organometallic compd. of Ge, Sn or Pb as catalyst is terminated at a desired degree of conversion of the monomer by addn. of a peroxide, e.g. H2O2, cumyl hydroperoxide, cyclohexanone peroxide, or tert-Bu hydroperoxide, which are supplied in an amt. of 0.001-5 parts by wt. per 100 parts by wt. of monomer. The pH of the reaction mixt. is brought to <4 after addn. of the peroxide. A perfectly white polymer is obtained and discoloration by the presence of traces of the Ce salt is prevented. The polymer has a high crystallinity, a syndiotactic index of 2-2.8, and a mol. wt. of 20,000-200,000, and is suitable for the prepn. of fibers, films, and tubes resistant to boiling water and chlorinated solvents. For example, a mixt. of 500 g. anhyd. vinyl chloride, 3.2 ml. Et4Pb, and a soln. of 0.9 q. cerium ammonium nitrate in 120 ml. MeOH was polymerized in a N atm. at -40.degree.. After 2 hrs. and 45 min., a soln. of 0.4 ml. 35% H2O2 and 0.3 ml. concd. HNO3 in 30 ml. MeOH was supplied and the polymerization stopped immediately. When H2O2 was added, no after-polymerization took

ANSWER 209 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:18894 CAPLUS

DOCUMENT NUMBER: 66:18894

TITLE: Copolymerization of vinyl chloride and ethylene

initiated by trialkylboron-peroxide catalyst systems

AUTHOR(S): Misono, Akira; Uchida, Yasuzo

CORPORATE SOURCE: Univ. Tokyo, Tokyo, Japan SOURCE: Bull. Chem. Soc. Jpn. (1966), 39(11), 2458-63

CODEN: BCSJA8

DOCUMENT TYPE: Journal LANGUAGE: English

Low-pressure copolymerization of vinyl chloride and ethylene is initiated AΒ by trailkylboronperoxide catalyst systems in a 1:1 water-MeOH mixt. at 0.degree.. In the presence of cocatalysts hydroperoxide, Et3P and Bu3B are active, while Ph3B is not. As cocatalysts, hydroperoxides, such as tert-BuOOH and cumene hydroperoxide, are more active than disubstituted peroxides such as Bz202, tert-Bu00B, and tert-Bu202, and azobis(isobutyronitrile). The highest catalytic activity is observed when the cocatalyst/catalyst mole ratio is 0.4. The initiating radical is suggested to be the hydroxy radical, and the initiating mechanism is discussed. The yield and the reduced sp. viscosity of the copolymer decrease rapidly with an increase in the ethylene content of the monomer mixt. The monomer reactivity ratios are: .gamma.1 (vinyl chloride) = 4.16 and .gamma.2 (ethylene) = 0.05. The copolymerization proceeds via a normal radical mechanism. The resulting copolymer shows characteristic ir absorption at .nu. 750 cm. -1 and N.M.R. at 8.37 .tau..

=> d his

L4

(FILE 'HOME' ENTERED AT 14:39:42 ON 06 SEP 2002)

FILE 'CAPLUS' ENTERED AT 14:40:04 ON 06 SEP 2002 L1 3 S FREEZING POINT DEPRESSION (3W) LIQUID

FILE 'BEILSTEIN' ENTERED AT 14:41:56 ON 06 SEP 2002 L2 2 S CUMENE HYDROPEROXIDE/CN

FILE 'CAPLUS' ENTERED AT 14:45:59 ON 06 SEP 2002

FILE 'REGISTRY' ENTERED AT 14:46:08 ON 06 SEP 2002 L3 1 S CUMENE HYDROPEROXIDE/CN

FILE 'CAPLUS' ENTERED AT 14:46:33 ON 06 SEP 2002 819 S L3 AND (WATER OR H2O OR AQUEOUS)

L5 375 S L4 AND (MIXTURE OR COMPOSITION)

L6 256 S L5 AND 1%

L7 0 S L5 AND WEIGHT PERCENT

L8 0 S L5 AND PERCENT WATER

L9 209 S L5 AND % WATER

=> s 19 and cumene/ti

2000 CUMENE/TI 22 CUMENES/TI

2022 CUMENE/TI

((CUMENE OR CUMENES)/TI)

L10 16 L9 AND CUMENE/TI

=> d ibib abs 1-16

L10 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 2002:429321 CAPLUS

DOCUMENT NUMBER: 136:403494

TITLE: Process for separating phenol from a mixture

comprising at least hydroxyacetone, cumene,

water and phenol

INVENTOR(S): Schwarz, Christoph; Weber, Mark; Tanger, Uwe; Korte,

Hermann-Josef; Ullrich, Jochen

PATENT ASSIGNEE(S): Phenolchemie G.m.b.H. & Co. K.-G., Germany

SOURCE: U.S. Pat. Appl. Publ., 9 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent English

LANGUAGE:

KIND DATE

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.

```
-----
                                                              -----
                     A1 20020606 US 2001-970856 20011005
A1 20020613 WO 2001-EP14029 20011130
     US 2002066661
     WO 2002046133
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
             UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:
                                        DE 2000-10060505 A 20001206
     Phenol is sepd. from a mixt. contg. hydroxyacetone, cumene,
     H2O and phenol, by fractionating the mixt. in a process
     with a fractional distn. step and a phase sepn. step to provide a single
     phenol fraction contg. <300 ppm of hydroxyacetone. In the work-up by
     distn. of cleavage product mixts., the hydroxyacetone can be
     removed from the cleavage product mixt. together with a phenol
     fraction from which the hydroxyacetone has to be removed. A process can
     be used for purifying cleavage product mixts. obtained in the
     cleavage of alkylaryl hydroperoxides such as cumene hydroperoxide.
     process allows sepn. of phenol and acetone from mixts. obtained
```

L10 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2002 ACS

in the cleavage of cumene hydroperoxide.

ACCESSION NUMBER:

2002:256835 CAPLUS

DOCUMENT NUMBER:

136:296542

TITLE:

Decomposition of cumene oxidation product

INVENTOR(S):

Hertzog, Richard R.; Sifniades, Stylianos; Fisher,

William Bernard

PATENT ASSIGNEE(S):

SOURCE:

U.S. Pat. Appl. Publ., 8 pp., Cont. of U.S. Ser. No.

APPLICATION NO. DATE

601,879.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION N	Ο.	DATE
US 2002040165	A1	20020404	US 2001-865190		20010723	
PRIORITY APPLN. INFO.	:		US	1989-297333	В1	19890117
			US	1992-920811	В1	19920724
			US	1994-203845	B1	19940228
			US	1994-333929	B1	19941103
			US	1996-601879	A1	19960215

A process for decompg. a cumene oxidn. product mixt. contg. AB cumene hydroperoxide (CHP) and dimethylphenyl carbinol (DMPC) to produce phenol, acetone and alpha-Me styrene (AMS) with enhanced safety of operation and reduced byproduct formation comprises the steps: (a) mixing the cumene oxidn. product in a stirred or back-mixed reactor with an acid catalyst, with 10-100 % acetone relative to the amt. of acetone produced during the decompn. reaction, and with up to 4% addnl. amts. of water relative to the reaction mixt., at an av. temp. between about 50-90.degree. for a time sufficient to lower the av. CHP

concn. of the reactor to 0.2-3.0%, and wherein a portion of DMPC is converted to dicumyl peroxide (DCP); then (b) reacting the reaction mixt. from step (a) at a temp. between about 120-150.degree. under plug-flow conditions for a time sufficient to decomp. substantially all residual CHP and at least 90% of the DCP formed in step (a).

L10 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:785348 CAPLUS

DOCUMENT NUMBER: 135:305480

TITLE: Cumene hydroperoxide production process

INVENTOR(S): Zakoshanskii, V. M.; Gryaznov, A. K.; Vasil'eva, I. I.

PATENT ASSIGNEE(S): Russia

SOURCE: Russ., No pp. given

CODEN: RUXXE7

DOCUMENT TYPE: Patent LANGUAGE: Russian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
RU 2146670 C1 20000320 RU 1998-108236 19980429

AB Emulsion-free two-stage air oxidn. of cumene in absence of initiators, catalysts, additives, and alkali agents in at least two reactor system is described. In the first reactor, cumene conversion at temp. up to 111-95.degree. is maintained at the level of at least 16%. Process is carried out in countercurrent reactor using pure alkali-free cumene. Oxidn. products from the first-stage are treated with ammonium hydroxide soln. until pH at least 8 is reached. When two or more second-stage reactors are available, oxidn. products are treated in each subsequent rector of the system. Conversion of cumene in the second oxidn. stage is maintained at up to 25 wt % at temp. at least 100-85 C, oxidn. charge and oxidizing agent being supplied concurrently. In all first- and second-stage reactors, pressure is maintained at least 4 atm and molar ratio of supplied oxygen to maximally consumed oxygen is maintained within a range of 1.12-1.30. Oxidn. products from the last second-stage oxidn. reactor are distd. to give industrial-grade (63-93%) cumene hydroperoxide. Excessive cumene is returned into process to be treated with aq. ammonium soln. to pH 9-10. Recycle cumene from hydrogenation stage and fresh cumene are treated with mixt. of 5-10% aq. NaOH soln. and 5-10-% aq. sodium carbonate soln. Combined streams of the above-mentioned cumenes are washed with water at cumene-towater ratio 1: (0.15-0.20). Concn. of cumene hydroperoxide in product rises with rate 2.5 to 4.5% per h, while selectivity is not below 94 mol % and cumene conversion 21-22 mol %.

L10 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:45962 CAPLUS

DOCUMENT NUMBER: 134:86026

TITLE: Isopropylation process and zeolite catalysts for the

manufacture of **cumene** from benzene and isopropanol or propylene and isopropanol

INVENTOR(S): Cappellazzo, Oscar; Girotti, Gianni; Pollastri,

Massimiliano; Lombardini, Sergio; Piccininno, Domenico

PATENT ASSIGNEE(S): Enichem S.p.A., Italy SOURCE: Eur. Pat. Appl., 29 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

A1 20010117 EP 2000-202434 20000710 EP 1069100

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO

IT 99MI1531 A1 20010115 IT 1999-MI1531 19990713

JP 2001055351 A2 20010227 JP 2000-212526 20000713 PRIORITY APPLN. INFO.: IT 1999-MI1531 A 19990713

OTHER SOURCE(S): CASREACT 134:86026

Benzene is isopropylated into cumene by its reaction with isopropanol or a mixt. of isopropanol and propylene in the presence of a catalyst comprising a zeolite and an inorg. ligand and the isopropylation is conducted under temps. and pressures such that the concn. of water

in the reaction's liq. phase is .ltoreq.8000 ppm, regardless of the total water content in the reaction mixt. The cumene may

subsequently be oxidized into cumene hydroperoxide, reacted with an acid to form phenol and acetone, and the acetone hydrogenated into isopropanol.

REFERENCE COUNT: THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS 3 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:410363 CAPLUS

DOCUMENT NUMBER:

TITLE: Installation and process for decomposition of

cumene hydroperoxide for phenol manufacture in

inert solvents

133:19089

INVENTOR(S): Anastasiu, Valentin; Vintan, Lucian; Lupascu, Mihai;

Botoc, Gheorghe; Paduraru, Dan-Mugurel; Gradinaru, Apostol; Strapuc, Valentin; Constantinescu, Victoria;

Murarasu, Liliana

PATENT ASSIGNEE(S): S.C. Carom S.A., Onesti, Rom.

SOURCE:

Rom., 7 pp. CODEN: RUXXA3

DOCUMENT TYPE: Patent

LANGUAGE: Romanian

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

KIND DATE PATENT NO. APPLICATION NO. DATE ----------RO 1995-1717 19951002 RO 111185 B1 19960730

The tech. grade cumene hydroperoxide decomps. in one step in acetone as AB inert solvent, forming an acetone-phenol mixt. with mol. ratio of 1.1-1.6:1, acidity of 0.08-0.12%, preferably 0.09-0.1%, at 56-60.degree. and atm. pressure and without addn. of water. The app. comprises tubular heat exchanger tubular reactor equipped with baffles to promote heat transfer and control of the reaction temp., inlet and outlet valves, recirculation pumps, pump control sensors for reactants, and pumping system for sulfuric acid. The installation of the invention was used in decompn. of cumene hydroperoxide and of dicumyl peroxide, using H2SO4, producing phenol-acetone mixt.

L10 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2002 ACS

1991:249743 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 114:249743

TITLE: Purification of acetone for regeneration of sorption

beds for treatment of wastewater from production of

phenol from cumene hydroperoxide

INVENTOR(S): Bogdaniak-Sulinska, Wanda; Zieborak, Kazimierz;

Galbfach, Ryszard; Zebrowski, Michal; Rosciszewski, Andrzej; Dudek, Joanna; Mlynarczyk, Anna; Franek,

Lucjan

PATENT ASSIGNEE(S):

Instytut Chemii Przemyslowej, Pol.

SOURCE: Pol., 5 pp. Abstracted and indexed from the unexamined

> application. CODEN: POXXA7

DOCUMENT TYPE: Patent LANGUAGE: Polish

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

AUTHOR (S):

PATENT NO. KIND DATE APPLICATION NO. DATE ----------PL 152006 B1 19901031 PL 1987-266435 19870625

Shaking impure Me2CO obtained along with phenol in the acid decompn. of AB cumene hydroperoxide with 5-15% addnl. water and withdrawing the upper hydrocarbon layer gave Me2CO contg. <30% water, useful for the title process. Thus, a mixt. contg. Me2CO 69.23, phenol 0.33, mesityl oxide (I) 0.006, cumene 0.22, .alpha.-metylstyrene (II) 4.55, acetophenone (III) 0.01, and water 19.65% was shaken 30 s with 5% addnl. water, and after 15 min aging, a lower layer contg. Me2CO 74.18, phenol 0.01, I 0.003, cumene 0.8, II 0.5, III 0.007, and water 24.5% formed.

L10 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:514518 CAPLUS

DOCUMENT NUMBER: 113:114518

TITLE: Kinetic characteristics of decomposition of

cumene hydroperoxide in solutions of

perchloric acid in water-alcohol solvents Vinnik, M. I.; Kislina, I. S.; Bushmakin, L. G.

Inst. Khim. Fiz. im. Semenova, Moscow, USSR CORPORATE SOURCE:

Kinet. Katal. (1990), 31(3), 528-34 SOURCE:

CODEN: KNKTA4; ISSN: 0453-8811

DOCUMENT TYPE: Journal LANGUAGE: Russian

PhCMe2OOH (I) hydrolysis to PhCMe2OH and H2O2 and its decompn. to PhOH and AB

Me4CO were studied in HClO4-contg. ROH-H2O (R = Et, Pr, Me3C) mixts. The yield of PhOH and Me2CO decreased with increasing

HClO4 concn. PhOH and Me2CO were formed by 2 paths, 1 involving a I

complex with H3O+ ClO4-. H2O and the other a I-H5O2+ complex.

L10 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:157487 CAPLUS

DOCUMENT NUMBER: 112:157487

TITLE: Kinetics of cumene hydroperoxide

> decomposition in aqueous solutions with catalysis by perchloric acid and hydrochloric

acid-alkali metal chloride mixtures

AUTHOR (S): Kislina, I. S.; Bushmakin, L. G.; Sysoeva, S. G.;

Antonovskii, V. L.; Zakoshanskii, V. M.; Vinnik, M. I.

CORPORATE SOURCE: Inst. Khim. Fiz., Moscow, USSR SOURCE:

Kinet. Katal. (1989), 30(1), 229-32

CODEN: KNKTA4; ISSN: 0453-8811

DOCUMENT TYPE: Journal LANGUAGE: Russian

Two mechanisms for the title process were found. In the first, the rate const. is proportional to the deriv. of the thermodn. activities of acid

and water and is identical for K+, Na+, and Li+ solns. In the second, the rate const. is proportional to the concn. of H502+...

L10 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1987:120376 CAPLUS

DOCUMENT NUMBER: 106:120376

TITLE: Method of .alpha.-methylstyrene isolation from

byproducts arising during phenol production by the

cumene process

INVENTOR (S): Koval, Jan; Mikula, Oldrich; Revus, Milos; Komorova,

> Hana; Brezula, Ludovit; Stefanik, Ivan; Tatransky, Ivan; Krizka, Pavel; Danilla, Frantisek; Suva, Jan

PATENT ASSIGNEE(S): Czech.

Czech., 5 pp. SOURCE:

CODEN: CZXXA9

DOCUMENT TYPE: Patent Slovak LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE PATENT NO. KIND DATE CS 234827 B1 19850416 CS 1983-4241 ______ CS 234827 19830613

AB Increasing the water content of a mixt. of the title byproducts (aliph. and arom. ketones, alcs., and heterocyclics) from the usual 1.5 to 14% enables sepn. of an azeotropic mixt. of Me2CO, PhCMe: CH2 (I), cumene, water, and minor amts. of PhOH and PhCOMe at the column head, and crude PhOH discharge at the base. The head product is distd. in a second column with added NaOH, Me2CO is sepd. at the head, and PhONa is removed from the aq. phase. The org. phase is fractionated in a third column at 6-19 kPa and reflux ratio 10 to give pure cumene which is recycled into the oxidn. process, and a mixed cumene-I fraction which is hydrogenated. The reflux ratio is then changed to 6 to yield pure (>98%) I and distn. bottoms contg. dimers of I and PhCOMe which are collected and worked up sep.

L10 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:7928 CAPLUS

DOCUMENT NUMBER: 82:7928

Catalytic activity of some silica-alumina-TITLE:

water (n SiO2.m Al2O3.xH2O) systems on the

decomposition reaction of cumene

hydroperoxide. IV. Infrared study of synthetic

systems of aluminosilicates Cormos, Liviu; Popica, Stana

AUTHOR (S): CORPORATE SOURCE: Rom.

SOURCE: Stud. Univ. Babes-Bolyai, Ser. Chem. (1974), 19(1),

19-24

CODEN: SUBCAB

DOCUMENT TYPE: Journal LANGUAGE: English

The ir spectrum of aluminosilicates was studied, in relation to their use as catalysts in decompn. of cumene hydroperoxide. Shifts of the ir bands

in relation to compn. are given and correlated with the max. catalytic activity of aluminosilicates contg. 30% Al203. Mech. mixts. of Al2O3 and SiO2, which are noncatalytic were also

studied.

L10 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1973:58042 CAPLUS

DOCUMENT NUMBER: 78:58042

Removing sulfuric acid from mixtures arising TITLE:

from the acid fission of cumene

hydroperoxide

Boehme, Guenter; Kiessling, Wolfgang; Moll, Karl INVENTOR(S):

Klaus; Raue, Bernd Ger. (East), 4 pp.

SOURCE:

CODEN: GEXXA8

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE PATENT NO. KIND DATE 19720805 DD 1971-153765 19710315 DD 91643

The title process involves extn. with a small amt. of water and AB eliminates the need for neutralization of the mixt. and subsequent deposition of salts in distn. columns. Thus, a cumene hydroperoxide decompn. mixt. contg. cumene 0.80, PhCOMe 0.95, Me2PhCOH 0.05, **H2O** 0.60, Me2CO 34.90, .alpha.-methylstyrene (I) 1.10, PhOH 57.45, higher phenols 2.10, I dimer 0.60, phenol tar 1.20, mesityl oxide 0.15, and H2SO4 0.10 wt. % was treated countercurrently at 4 1./hr in an extn. column filled with Raschig rings with 1 l./hr H2O at 40.degree. (theor. step no. 0.24) to give a mixt. contg. <10 mg/l. H2SO4. Eight further examples illustrated changes in extn. conditions.

L10 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:445113 CAPLUS DOCUMENT NUMBER: 73:45113

Removal of salts from phenol and acetone obtained by TITLE:

decomposition of cumene hydroperoxide

Janda, Jan; Koval, Jan; Kukel, Jan INVENTOR(S):

SOURCE: Czech., 3 pp. CODEN: CZXXA9

DOCUMENT TYPE: Patent Czech

LANGUAGE: FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
CS 131559 19690315 CS 19670 19670209

AB Requisite conditions are described which reduce the content of inorq. salts in the org. phase <0.01% and prevent clogging of the boiler and column. Thus, a mixt., after acid hydrolysis of cumene hydroperoxide, contg. 3 kg AcH, 2656 kg Me2CO, 55 kg mesityl oxide, 56.2 kg cumene, 215.3 kg PhCMe:CH2, 3935.6 kg PhOH, 41.5 kg PhCOMe, 115.2 kg cumenylphenol, 14.7 kg Me2CPhOH, 357.8 kg pitch, 5.6 kg H2SO4, and 50.5 kg H2O, was homogenized at 55.degree. with a soln. prepd. from PhONa and phenol water, contg. 203.5 kg PhONa, 402.7 kg PhOH, 14.9 kg Me2CO, 3.7 kg PhCOMe, 5.6 kg p-cumylphenol, and 1545.5 kg H2O. The mixt. was treated at 55.degree. with 85.3 kg 94% H2SO4 to give 2 layers in 30 min. The upper org. layer contained all org. substances, 12% H2O, and 0.008% Na2SO4, while the lower aq. layer contained 25% Na2SO4, 0.3% PhOH, and 0.6% Me2CO. The content of Na3SO4 in the org. phase dropped to 8% and the Na salts of org. acids passed into the aq. layer.

L10 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:78664 CAPLUS

DOCUMENT NUMBER: 72:78664

TITLE: Continuous catalytic cleavage of cumene

hydroperoxide with sulfuric acid Mantegazz, Attilio; Reni, Cesare

INVENTOR(S): PATENT ASSIGNEE(S): Societa Italiana Resine S.p.A.

SOURCE: Ger., 5 pp. CODEN: GWXXAW

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE DE 1443330 DE 1443329 19700102

PRIORITY APPLN. INFO.: IT 19620110

Cumene hydroperoxide (I) is converted to phenol (II) and acetone (III) by homogeneous catalytic cleavage with H2SO4 in a heat-exchanger to remove

the reaction heat. Thus, 500 parts of a previous cleavage mixt. is recycled with a pumpto a velocity of 2 .times. 105 parts/hr. The heat-exchanger is fed with H2O at 90.degree. until the recycled mixt.reaches 70.degree., then it is cooled with water at 25.degree. I (81.9% in cumene) 1000 parts/hr and 98% H2SO4 2 parts/hr is added continuously to the recycled flow (ratio 1:217), while 1002 parts/hr reaction mixt. is removed continuously from the system. The concn. of I never exceeds 0.1% during the reaction, the temp. is kept at 70-2.degree. at normal pressures. The product mixt. is neutralized by ion-exchangers and the products are sepd. by distn. yielding 98% II and 96% III.

L10 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:410222 CAPLUS

DOCUMENT NUMBER: 69:10222

TITLE: Separation of cumene hydroperoxide

decomposition products

INVENTOR(S): Nixon, Joseph R., Jr.

PATENT ASSIGNEE(S): Hercules Inc. SOURCE: U.S., 5 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 3365375 A 19680123 US 1965-448414 19650415

The products obtained by catalytic decompn. of cumene hydroperoxide are AB sepd. by distn. in a distn. tower divided into 2 zones of approx. equal size by a horizontal baffle plate. Substantially pure acetone contg. .ltoreq. 1% water is withdrawn from the head of the column, hydrocarbons and water, both free of acetone and phenol, are withdrawn from an intermediate point of the column, and phenol contq. small amts. of water, heavy ends, and hydrocarbons is withdrawn from the base of the column. The acetone and hydrocarbon fractions are suitable for use in subsequent operations without further purification. The distn. process is economical because only a single distn. tower is required. Thus, 100 parts/hr. of catalyst-free cumene hydroperoxide decompn. product comprising acetone 45.3, water 11.6, hydrocarbons 4.8, phenol 35.6, and heavy ends 2.7% is introduced at the midpoint of a distn. column contg. 55 plates and sepd. in the center by a baffle plate. Live steam is also introduced at 8.6 parts/hr. at the column midpoint, and high pressure steam is introduced at 67 parts/hr. to the base of the distn. column. The amt. of steam used was equiv. to 1944 Btu./lb. of acetone introduced and sepd. A ratio of 4 parts of reflux/part of distillate removed at the column head is employed. Acetone, contg. <1% water, is removed at 44.3 parts/hr. from the column head. A mixt. of hydrocarbons and water is recovered from the midpoint of the distn. column. The mixt. is sepd. by decantation, and 4.6 parts/hr. hydrocarbons and 16.9 parts/hr. water are recovered, while 46 parts/hr. hydrocarbons and 19.5 parts/hr. water are returned as reflux. A mixt. of phenol 86.2. water 6.8, hydrocarbons 0.5, and heavy ends 6.5% is recovered from the bottom of the distn. column at the rate of 41.3 parts/hr. The acetone product contained no traces of phenol and could be recycled for use in the catalytic decompn. of cumene hydroperoxide.

L10 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1968:108273 CAPLUS

DOCUMENT NUMBER: 68:108273

TITLE: Catalytic activity of nSiO2.mAl2O3.xH2O systems in the

decomposition reaction of cumene

hydroperoxide. I

AUTHOR(S): Pop, Augustin; Krobl, Paul; Cormos, Liviu; Lengyel,

Gheorghina

CORPORATE SOURCE: Univ. " Babes-Bolyai", Cluj, Rom

SOURCE: Stud. Univ. Babes-Bolyai, [Ser.] Chem. (1967), 12(2),

89-95

CODEN: SUBCAB

DOCUMENT TYPE: Journal LANGUAGE: Russian

The systems nSiO2.mAl2O3.xH2O (where n = 0-20, m = 0-5, and x = 0-3 at 420 and 580.degree. activation temp.) were prepd. by copptg. the mixed gels in proportions desired, from a soln. contg. free silicic acid and Al(NO3)3, at room temp., adding gradually (NH4)2CO3 soln.; a voluminous gel formed at pH .apprx.5. The filtered ppt. is left to dry in free air for several days, is dried at 105.degree., is ground and classified, and is heat-treated. The compn. obtained ranged from 100% SiO2 to 100% Al2O3. D.T.A. and differential thermogravimetric anal. curves (10.degree./min., in air) showed that absorbed H2O is removed at <350.degree., with max. rate at 130.degree., most of the water of crystn. is removed at <700.degree., with the max. rate at 460-70.degree., and the remainder is removed at <1000.degree. at a const. rate. No addnl. modifications were indicated at <550.degree., but at <550.degree. the establishment of chem. bonds between the 2 oxides were indicated, concomitant with elimination of the last amts. of H2O . The optimal activation temps. were 420.degree. (where the water of crystn. removal was min.) and 580.degree. (where the water of crystn. removal became const.). The sp. surface decreased with increase of the Al2O3 proportion from 423 m.2/g. at 0% Al2O3, to 291 m.2/g. at 84.9% Al2O3. The catalytic properties of the systems were studied by using cumene hydroperoxide (I) decompn. as a reaction model. The expts. were effected in a static-type glass reactor, with internal and external cooling (most perfect cooling is essential to remove the reaction heat under isothermal conditions). In each expt. 21 g. of a 10% I soln. was treated with 2.2 g. catalyst, at 20, 30, and 40.degree., agitating strongly. The unconverted I was detd. iodometrically. For the 2 systems with m = 4, n = 1 and with m = 2.5, n = 1, the sp. reaction rate consts. were: at 20.degree. 0.093, 0.04; 30.degree. 0.21, 0.08; 40.degree.-0.37, 0.16; the resp. activation energy values were 12.5 and 12.4 kcal./mole. Examn. of the variation of the conversion as function of the system compn. and of the temp. of activation and of reaction, showed that max. conversion was obtained for the system with m = 3, n = 1; the conversion increased with both temps., obtaining 94% at 40.degree..

L10 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:422479 CAPLUS

DOCUMENT NUMBER: 67:22479

TITLE: Unsaturated polyester curing system consisting of

cumene hydroperoxide, methyl ethyl ketone

peroxide, and thioglycolic acid

INVENTOR(S):
Montesano, Lewis

PATENT ASSIGNEE(S): Bell Telephone Laboratories, Inc.

SOURCE: U.S., 2 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
US 3318974 19670509 US 19650323

AB Styrene-polyester (I) is cured with a critical mixt. of free-radical initiators. Thus, 100 parts I, viscosity 600-750 cp., sp. gr. 1.11-1.13, a 7:3 mixt. of a polyester from phthalic

anhydride, maleic anhydride, and propylene glycol with styrene, was thoroughly mixed with cumene hydroperoxide 0.25, Me Et ketone peroxide 0.5, and thioglycolic acid (II) 0.5 part. After 5 min. at room temp. the mixt. had gelled to form a water-white hard resin without cracks. The same results were obtained with 0.25 parts II.